CRANFIELD UNIVERSITY

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Bioaerosol emissions from open windrow composting facilities: Emission characterisation and dispersion modelling improvements

School of Applied Science
PhD

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Academic Year: 2012 - 2013

Supervisors: Dr Gill Drew and Dr Sean Tyrrel
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This thesis is submitted in partial fulfilment of the requirements for the degree of PhD

ABSTRACT

Bioaerosol emissions from open windrow composting facilities are becoming of increasing concern due to the negative health effects associated with bioaerosols, and the fact that emissions from open windrow facilities are not contained. Current bioaerosol monitoring techniques provide only a snapshot of bioaerosol concentrations spatially and temporally, whereas dispersion models have the potential to offer a more continual overview of bioaerosol levels, alongside existing sampling methods. However, dispersion models have not been successful at accurately predicting bioaerosol concentrations from open windrow composting facilities, generally under predicting concentrations by at least one order of magnitude. This is predominantly due to a lack of knowledge and data surrounding the complex nature of bioaerosol release and transportation, particularly when the compost is agitated. This study aimed to improve the reliability in the outputs of the ADMS dispersion model, specifically in the open windrow composting scenario, by performing several model tests alongside selected input parameter quantification improvements. This involved completing a sensitivity analysis, and a model calibration and validation specific to this scenario for the first time. Results from the sensitivity analysis showed that the use of wet and dry deposition modules is significant, and the majority of model inputs associated with the representation of the source of the emission are sensitive. These findings helped select the model input parameters for quantification improvements. Novel preliminary measurements of bioaerosol temperature, velocity and concentration at the source of composting agitation activities were completed. These values provided more accurate model inputs. Collectively, these results allowed the model to be successfully calibrated, and consequently, validated for the first time for this specific scenario, resulting in model outputs corresponding to within one order of magnitude to measured data. This has helped to generate an initial set of modelling recommendations, allowing modellers to use the ADMS dispersion model in a reliable manner, when applied to the open windrow composting scenario. Eventually, these improved model outputs may be used to predict bioaerosol exposure levels at sensitive receptors, particularly in conditions where current monitoring methods are not feasible.

For my mother and father, Lorraine and Stephen Douglas

Thank you for all the sacrifices you have made over the years, and for the support and encouragement you have given me

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LIST OF ABBREVIATIONS

ADMS	Atmospheric Dispersion Modelling System
AERMIC	AMS/EPA Regulatory Model Improvement Committee
AfOR	Association for Organics Recycling
AFS	Aerosol Fluorescence Sensor
ANCOVA	Fixed Analysis of Covariance
CALPUFF	California Puff Model
CERC	Cambridge Environmental Research Consultants
CFD	Computational Fluid Dynamics
CFU	Colony Forming Units
EA	Environment Agency
EF	Modelling Efficiency
EPA	Environment Protection Agency
F	F-Test
FAST	Fourier Amplitude Sensitivity Testing
FB	Fractional Bias
FEL	Front End Loader
GLM	General Linear Model
GPS	Global Positioning System
HDMR	High Dimensional Model Representation
ISC	Industrial Source Complex
IVC	In-Vessel Systems
LLOD	Lower Limit of Detection
LSD	Least Significant Difference
M	Mean Difference
MAC	MacConkey Agar
MBT	Mechanical Biological Treatment
MC	Monte Carlo
MEA	Malt Extract Agar
MMOL	Minimum Monin-Obukhov Length
NA	Nutrient Agar
OAT	One-at-a-Time
r	Correlation Coefficient

r^2	Coefficient of Determination
rANOVA	Repeated Measures Analysis of Variance
RAT	Reflected Apparent Temperature
RI	Regulars Image
RMSE	Root Mean Square Error
SA	Sensitivity Analysis
SEM	Standard Error of the Mean
SGC	Significant Gradient Change
SSBRA	Site Specific Bioaerosol Risk Assessment
TI	Thermal Image
TIC	Thermal Imaging Camera
UV	Ultra Violet
VOC	Volatile Organic Compound
WIBS	Wide Issue Bioaerosol Sensor

1 Project overview, introduction and aim

The volumes of material being composted are increasing due to European legislation (European landfill directive [1999/31/EC], Sykes *et al.,* 2007). Composting is the breakdown of organic material via intense microbial activity (Adani *et al*., 1997; Boulter *et al.,* 2002; Chiang *et al.,* 2003) leading to the generation of high concentrations of microorganisms that can become aerosolised (ADAS and SWICEB, 2005). These aerosolised microorganisms and their associated cellular components are referred to as bioaerosols, and are ubiquitous in ambient air (Crook and Sherwood-Higham, 1997; Kummer and Thiel, 2008). Bioaerosols emitted from open windrow composting facilities are not controlled or contained, and are not easy to capture. Elevated levels of bioaerosols are found during open windrow composting agitation activities, such as turning screening and shredding (Taha *et al.,* 2006). One of the major concerns with bioaerosol release from composting facilities is the adverse health effects associated with exposure to the general public. However there is currently no clear evidence of the degree of exposure that the public working or living in the vicinity of open windrow composting facilities are subjected to, nor is there any firm evidence regarding the levels of bioaerosol required to instigate the onset of associated health problems (Douwes *et al.,* 2003). At present, the Environment Agency position statement on 'composting and potential health effects from bioaerosols' (Environment Agency, 2010), recommends that bioaerosol concentrations should be maintained to an acceptable level within 250 metres of the site boundary, or the nearest sensitive receptor, whichever is closer. These acceptable levels are currently set at 1000, 500 and 300 Colony Forming Units per cubic metre (CFU/m^3) for Total Bacteria, *Aspergillus fumigatus* and Gram-negative Bacteria, respectively (Environment Agency, 2010). At present, monitoring methods are only able to provide snapshots of emissions in space and time, and can only be used in specific weather conditions (AfOR, 2009). If used alongside current sampling methods, dispersion models have the potential to provide a more continuous overview of bioaerosol concentrations surrounding open windrow composting facilities. They also have the potential to be used to estimate:

- Bioaerosol emissions in a variety of operational scenarios and weather conditions.

  For example, bioaerosol concentrations can be estimated at the nearest sensitive receptor, or 250 metres from the site boundary, during certain agitation activities. This can determine whether certain agitation activities or combinations of agitation activity result in exceeding the acceptable levels of bioaerosol concentrations 250 metres from the site boundary or nearest sensitive receptor. This may influence the way a site is operated, to help manage the risks of exceeding the permitted bioaerosol levels.
- Levels of exposure to compost workers and the general public.

  As dispersion models have the potential to estimate continuous bioaerosol concentrations at defined locations, this information could be used to estimate the level of exposure at certain locations during specified time ranges. This information can further be used to address the gap in knowledge surrounding the link between bioaerosol exposure and the onset on bioaerosol-related illnesses.
- Possible future bioaerosol concentrations at locations where a new composting facility is proposed, or at existing facilities wishing to expand.

  At present, when sites apply for permits to expand, or when a company wishes to establish an open windrow composting facility, it is difficult for the site to demonstrate that bioaerosol concentrations will remain below the permitted bioaerosol concentration levels stipulated by the Environment Agency (Environment Agency, 2010). Dispersion models have the potential to provide an accurate estimation of the possible increased bioaerosol concentrations caused by the new facilities or expansions, thus aiding the permitting process.

However dispersion models have not yet been successful at estimating bioaerosol emissions from open windrow composting facilities (Drew *et al.,* 2007; Taha *et al.,* 2006; 2007). Dispersion models have been well-established at estimating 'traditional' airborne pollutants such as particulates (PM), NO_x, SO_x, CO_2, CH_4, and ozone (USEPA, 2010). Theoretically dispersion models

should be capable of accurately estimating bioaerosol emissions as they have been used with some success to predict odour dispersion and exposure at:

- Landfill sites (Sarkar *et al.,* 2003)

  Sarker *et al.* (2003) simulated odour emissions from Municipal Solid Waste [MSW] landfill sites using the dispersion model *COMPLEX-I*. Modelled outputs were used to create odour contour maps to analyse the variations in odour exposure to the nearby sensitive receptors, which were used to link this to annoyance.
- Wastewater treatment facilities (McIntyre, 2000; Witherspoon *et al.,* 2000)

  McIntyre (2000) details the use of the dispersion model, ISC3, to assess the area most likely to be affected by odour emissions from wastewater treatment facilities. Modelled outputs were compared with odour complaint records, and the limit of odour annoyance coincided well with the limit of complaints received.

  Witherspoon *et al.* (2000) used the dispersion model ISCST3 to model odour emissions around the vicinity of wastewater and sewage treatment works, in various operational scenarios. The modelled outputs were used to assess areas were odour concentrations are high, and understand where the source of the odour was. It was also used to model the impacts of different odour control systems, and the impact this would have on odour dispersal.
- Sewage treatment works (Gostelow *et al.,* 2004)

  Gostelow *et al.* (2004) used an integrated odour model, STEnCH, to model odours from sewage treatment works. STEnCH was used to provide an indicator for the probability of odour annoyance.
- Poultry production units and meat rendering plants (Dincer *et al.,* 2004; Sheridan *et al.,* 2004; Hayes *et al.,*2006)

  Dincer *et al.* (2004) compared modelled and measured odour concentrations at two meat rendering plants. The CALPUFF dispersion model was used. The correlation between the modelled and measured

data was good at both sites, as r^2 values of 0.86 and 0.94 were observed.

Sheriden *et al.* (2004) used the ISCST3 dispersion model to assess the effects of several odour abatement techniques at pig production units.

Hayes *et al.* (2006) also used the dispersion model ISCST3. In this study, ISCST3 was used to determine the impact of odour emissions from existing poultry production facilities. This, in combination with several odour annoyance criterions, was used to assess setback distances for new facilities.

The use of a dispersion model in the bioaerosols from open windrow composting context is advantageous to:

- Regulatory bodies, when evaluating current guidance and bioaerosol limits
- Researchers, to help them understand the levels of exposure at the sensitive receptors, to establish how much exposure result in negative health impacts
- Operators of facilities, when applying for permits to expand or establish new facilities

This has led to the overall aim of the project:

To improve the confidence in model outputs when using dispersion models to estimate bioaerosol concentrations downwind of emissions from open windrow composting facilities.

To fulfil this aim, key gaps in knowledge were identified and used to form the objectives of this research. Overall two key gaps in knowledge were identified, firstly:

- A lack of quantification, and thus justification, of selected model input values used within dispersion models, when simulating the open windrow composting scenario

A sensitivity analysis, specific to bioaerosol emissions from open windrow composting scenario, can be completed to determine which model inputs affect the model outputs the most. The results from this analysis can be used to provide an order of prioritisation when improving the quantification of selected input parameters. This forms objective 1:

O1. To perform a sensitivity analysis, specific to the bioaerosol emissions from open windrow composting facilities scenario, to determine which input parameters affect the model output concentrations the most.

The second key gap in knowledge is:

- The performance of dispersion models has not been fully tested, due to a lack of a consistent, extensive bioaerosol measurement dataset from open windrow composting facilities, to compare to modelled outputs

A consistent, extensive bioaerosol dataset collected from two different open windrow composting facilities is now available, and can be used to test the performance of dispersion models in the open windrow composting context. This forms objective 2:

O2. To complete a model calibration and validation, in the context of bioaerosol emissions from open windrow composting facilities, using existing sets of measured data.

Upon completion of objective 1 , the results from this analysis can be used to provide an order of prioritisation when improving the quantification of selected input parameters. This forms objective 3, which also addresses the first key gap in knowledge:

O3. To collect data, using novel techniques and existing data collection methods if possible, to improve the knowledge of selected dispersion model inputs, in the open windrow composting context, to provide more accurate modelled output concentrations.

Once these objectives have been fulfilled, knowledge surrounding the dispersion modelling of bioaerosol emissions from composting facilities will be

much improved. Additionally, the dispersion model will have been fully tested in the open windrow composting context, which will determine whether the dispersion model can be used with confidence in this specific scenario. The information gained from completing this study can be used to help future model users, when simulating this complex and unique situation. This forms objective 4:

O4. To create best-practise modelling recommendations when using dispersion models to accurately estimate bioaerosol emissions from open windrow composting facilities.

The aim and objectives and the order in which they are addressed in the thesis is conceptualised in Figure 1-1.

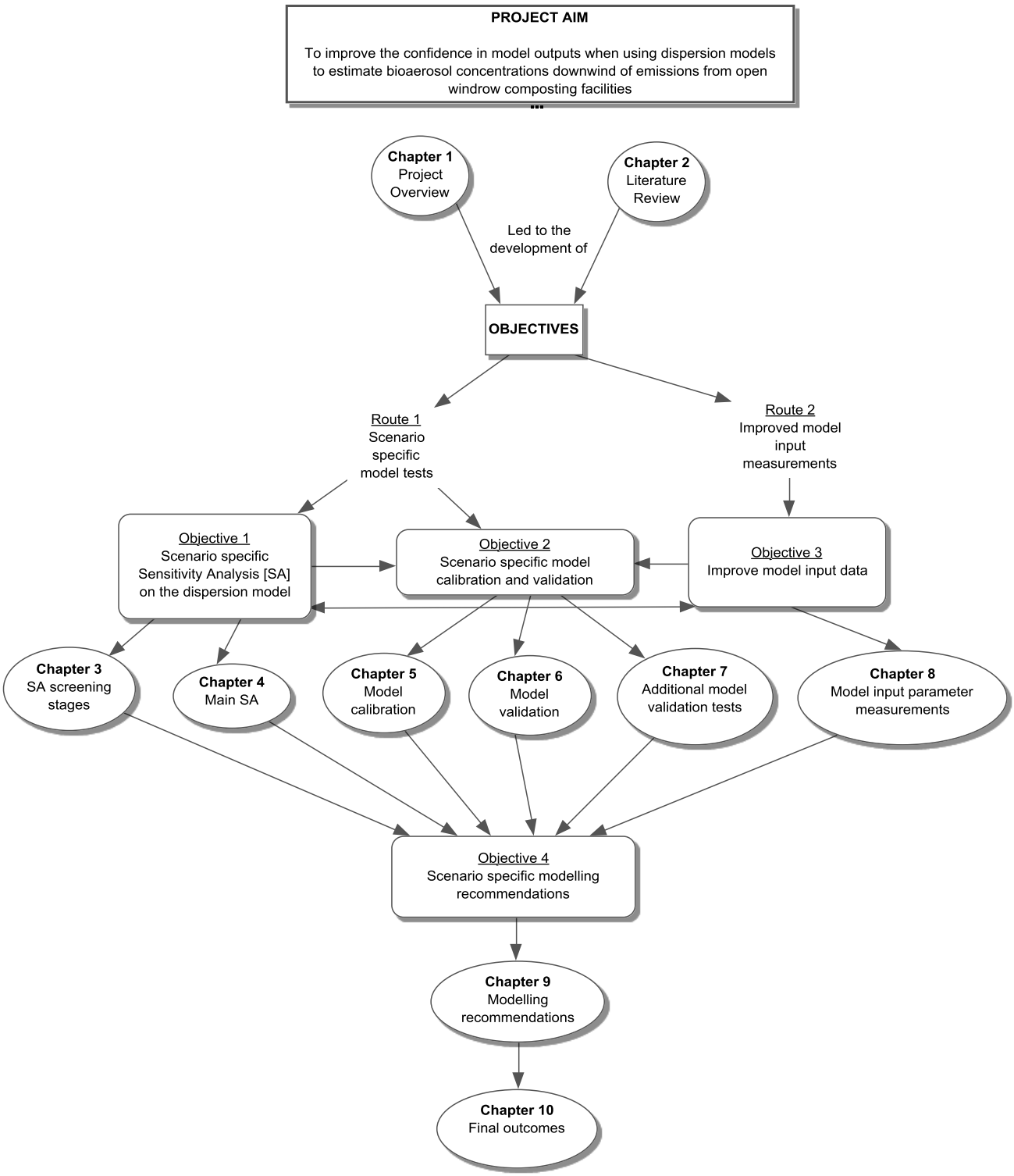

Figure 1-1 An overview of the structure of the thesis, highlighting where each object is addressed throughout the thesis, and how the objectives are interlinked.

Figure 1-1 shows how the objectives are interconnected. For example, the emerging results from completing objective 3 (Chapter 8) were used to influence decisions in when completing objectives 1 and 2 (Chapters 3-7) and vice versa. Although objective 3 is addressed towards the end of the thesis in Chapter 8, it should be appreciated that the work completed within this chapter shaped aspects of the work completed to fulfil other objectives which appear prior to this work.

The next chapter provides a more detailed background to composting, bioaerosols and dispersion models and critically reviews the progress made to date when modelling bioaerosols emitted from open windrow composting facilities. The main key gaps in knowledge and objectives are stated again, in more detail, within this chapter.

2 Literature review

2.1 Introduction

This chapter critically assesses the existing knowledge and literature surrounding composting, bioaerosols, and dispersion modelling of bioaerosols emitted from composting facilities, highlighting any gaps in knowledge. Extensive literature reviews have been completed prior to the commencement of this project, mainly focussing on bioaerosols and the composting process (Swan *et al.,* 2003; Taha 2005; Sykes *et al.,* 2007; Tamer Vestlund 2009; Pankhurst 2010). This chapter summarises the key points of the previous literature, and provides new insights regarding the work completed on the modelling of bioaerosols released from composting facilities.

2.2 Introduction to composting

2.2.1 Legislation

In 1999, the Council of the European Union issued the European landfill directive [1999/31/EC] (Council Directive, 1999). In summary, this document states that the amount of Biodegradable Municipal Waste [BMW] destined for landfill needs to be reduced so that at least 33% of household waste is recycled or composted by 2015 (DEFRA, 2009; European Commission, 2012). In the waste strategy for England, one of the main objectives was to meet and exceed the Landfill diversion targets for BMW in 2010, 2013 and 2020, (DEFRA, 2009). These targets are presented in Table 2-1.

Table 2-1 Landfill directive targets for BMW in England, adapted from DEFRA (2009)

Target Year	Landfill directive target	Amount of limit (tonnes)
2010	Reduce BMW landfilled to 75% of that produced in 1995	11.2 million
2013	Reduce BMW landfilled to 50% of that produced in 1995	7.4 million
2020	Reduce BMW landfilled to 35% of that produced in 1995	5.2 million

There are several strategic stages to reduce the amount of waste directed to landfill. This is referred to as the waste hierarchy (DEFRA, 2011), and is illustrated in Figure 2-1.

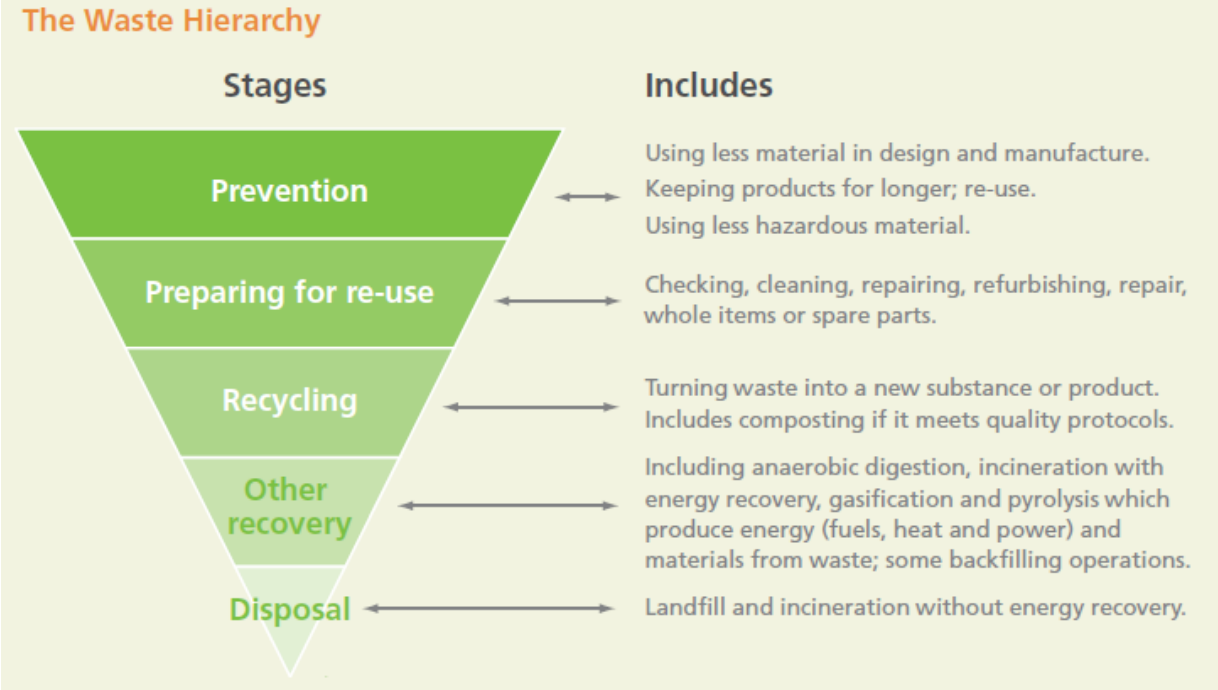

Figure 2-1 The waste hierarchy, highlighting the stages in place to reduce the amount of waste sent to landfill. Image duplicated from DEFRA (2011)

Figure 2-1 shows that composting is a key contributor to the reduction of waste sent to landfill, by recycling biodegradable waste to create a usable product. In 2010, the landfill directive targets were met as 40.3% of household waste was recycled, composted or re-used (Defra, 2011). To help achieve the targets

highlighted in Table 2-1, the number of composting facilities has increased, almost doubling in the UK between 2001/02 and 2003/4, (Slater *et al.,* 2005).

2.2.2 Types of composting facility

There are four main approaches to composting, as detailed in Swan *et al.,* (2003). These approaches are summarised below.

1. Windrow systems
    - Simple system used to compost mainly green waste, which consists predominantly of biodegradable garden waste, uncooked fruit and vegetables, wood and cardboard (SITA, 2013)
    - Green waste is formed into long piles called windrows
    - Windrows are usually open to the air, and thus pollutant emissions from this type of facility are uncontrollable
    - The windrows are turned regularly to allow air to blend into the waste, improving oxygen content and regulating temperature and moisture levels (WRAP, 2012)
2. Aerated static piles
    - Compost is not turned, but instead air is extracted or propelled through the material
    - This system is possible on open windrows, covered windrows and in closed containers
3. In-vessel systems [IVC]
    - This is an enclosed system, allowing greater control of emissions
    - The system can either be completed continuously, or in batches, depending on feed stocks and the type of system used.
    - Broadly, there are six types of in-vessel system:
        - Containers
        - Tunnels
        - Agitated bays
        - Rotating drums
        - Silos/tower systems
        - Enclosed halls

4. Vermicomposting
    - A lesser known type of composting in which selected species of earthworms are used to break down the feedstock
    - This is usually completed in long troughs at a temperature of 35°C.

Approximately 90% of composting facilities in the UK are open windrow systems, handling mainly green wastes (Sykes *et al.,* 2007). However it should emphasised that the number of IVCs are increasing, as a wider range of the biodegradable waste fraction can be composting using this method, including animal by-products, food and catering waste, in addition to green waste (IVC, 2013). IVCs are also able to control pollutant emissions, as well as the conditions of the composting process, consistently delivering high quality compost (IVC, 2013; SITA, 2013). As already highlighted, pollutant emissions from open windrow composting facilities are not controlled, as the composting windrow is constantly exposed to the atmosphere. Moreover, pollutant emissions are thought to be elevated during agitation activities (shredding, turning and screening), particularly as increased bioaerosol concentrations have been documented during these periods (Taha *et al.,* 2006).

Overall, this presents a challenge when modelling emissions from open windrow facilities, as emissions are not controlled and are difficult to characterise. This project focusses on open windrow composting facilities only, as this represents the most common facility in the UK, but also to address the challenges of modelling emissions this type of facility.

2.2.3 Open windrow composting process

Open windrow composting takes, on average, sixteen weeks to complete (WRAP, 2012). The composting process is usually comprised of three principal stages, shredding, the ‘main phase’ and screening (Swan *et al.,* 2003; WRAP, 2012), as detailed briefly below:

1. Prior to composting, the waste is usually shredded to a uniform size (WRAP, 2012). In some cases feed stocks are added to adjust carbon-to-nitrogen and moisture levels (Swan *et al.,* 2003).
2. The shredded waste is then formed into windrows. The windrow phase of composting is often referred to as the 'main phase'. During this phase, the windrows are turned often to improve oxygen content, and to regulate temperature and moisture levels (WRAP, 2012). The main phase can be further split into three stages (Swan *et al.,* 2003):
    a. High rate composting
        - High rate of biological activity
        - High heat generation
        - High demand for oxygen
    b. Stabilisation phase
        - Biological and heat activity starts to decline
        - Oxygen demand increases
        - Thermophilic temperatures are attained (>50ºC)
    c. Maturation phase
        - Further reduction in biological and heat generation
        - Oxygen demand decreases
3. At the end of the process, the material is screened to remove any contaminants and to grade the material into different sizes (WRAP, 2012)

During composting agitation activities such as turning, screening and shredding, bioaerosols are found in elevated levels, typically two to three orders of magnitude higher than concentrations measured during passive emissions (Taha *et al.,* 2006). Bioaerosol releases from agitation activities are uncontrollable, and are not easy to capture or measure, particularly as it is dangerous to sample close to the machinery that is used to agitate the compost.

2.3 Introduction to bioaerosols

2.3.1 Bioaerosol components and theirnegative health effects

Bioaerosols generated from composting facilities can consist of bacteria, constituents of cells, fungi, and pollen (Douwes *et al.,* 2003). The components of bioaerosols, and the species found at composting facilities are detailed in Table 2-2.

Table 2-2 A summary of bioaerosol components, and species found at composting facilities (Swan *et al.*, 2003; SWICEB, 2005; Le Goff *et al.,* 2010; Le Goff *et al.,* 2012)

Bioaerosol or bioaerosol component	**Species or components of bioaerosol found at composting facilities**
Fungi	*Cladosporium, Alternaria, Veticillum, Aspergillus, Eurotium, Penicillium, Trichoderma, Absidia, Mucor, Rhizopus,* Mycotoxins
Bacteria (Gram-negative), including endotoxin	*Pseudomonas, Klebsiella, Pantoea agglomerans, Rahnella, Alcaligenes,* endotoxin, *Actinetobacter, Enterobacter E.coli, Campylobacter, Salmonella*
Bacteria (Gram-positive)	*Corynebacteria, Bacillus, Staphylococcus, Micrococcus, Streptococcus,* Actinomycetes (see below)
Actinobacteria (Gram-positive) or Actinomycetes (old classification)	*Saccharopolyspora (faenia) rectivirgula, Saccharomonospora, Streptomycetes*
Glucans	(1→3)-β-D-glucan

Bioaerosol component sizes vary, from approximately 0.02 – 100 microns in diameter (Dowd and Maier, 2000). Smaller bioaerosol components, typically less than 10 microns in size, may not be filtered by the hairs in a human nose, and can penetrate deeply into the lung (Ivens *et al.,* 1999; Douwes *et al.,* 2003), which may cause adverse health problems.

Medical problems associated with bioaerosols are more likely to affect immune-compromised individuals (Epstein, 1996; HPA, 2011) and those regularly exposed to bioaerosols (Hansen *et al.,* 1997; Eduard *et al.,* 2012). Table 2-3 summarises some of the health effects associated with bioaerosols.

Table 2-3 A summary of some of the health effects caused by bioaerosols as detailed in Poulsen *et al.* (1995), Ivens *et al.* (1997), Douwes *et al.* (2003), Swan *et al.* (2003), Lorenz (2004), Harrison (2007), Srikanth *et al.* (2008), Domingo and Nadal (2009), HPA (2011), Corrao *et al.* (2012), and Hoppe *et al.* (2012)

	Health effects	**Agents**
Respiratory problems and diseases	Asthma, Rhinitis, Mucous membrane irritations, Chronic bronchitis, Tracheobronchitis, Airflow obstructions, Organic dust toxic syndrome, Farmer's lung, sinusitis, Aspergillosis	Fungi, Bacteria, Actinomycetes, Endotoxins, Glucans, Mycotoxins, Peptidoglycans, Microbial enzymes, Plant, mammalian and invertebrate proteins
Gastrointestinal problems	Diarrhoea and Nausea	Gram negative bacteria, Endotoxin, Fungi
Skin problems	Skin rash, Itching skin rash, Dermatitis, Dermatomycosis, Pyoderma, Eczema	Streptococci, Enterobacteria, Endotoxins

2.3.2 Legislation

There are currently no legal or exposure limits in place for the levels of bioaerosols emitted from composting facilities (Environment Agency, 2001). However, as bioaerosols can be harmful to human health, the Environment Agency [EA] does request that composting facilities complete a site specific bioaerosol risk assessment [SSBRA] as part of the environmental permitting process (Environment Agency, 2010). SSBRAs are used to assess whether bioaerosol levels will be maintained to acceptable levels at the 'sensitive receptors', such as a house or place of work (Environment Agency, 2010). The acceptable levels of bioaerosols are currently stated as:

- 1000 Colony Forming Units per cubic metre (CFU/m^3) for Total Bacteria

- 500 CFU/m^3 for *Aspergillus fumigatus*
- 300 CFU/m^3 for Gram-negative Bacteria

Bioaerosols must be monitored in accordance to the Association for Organics Recycling [AfOR] standardised protocol (AfOR, 2009; Environment Agency, 2010).

Bioaerosols have been referred to as pollutants (Pegas *et al.,* 2012; Vitezova and Vitez, 2013), contaminants (Adhikari *et al.,* 2011; Hsu *et al.,* 2012) and nuisances (Cré, 2004; Taha *et al.,* 2006) in the past. The US EPA (2011; 2013) defines an air pollutant to be threat to human or animal health, or have an adverse effect on the environment. The term 'nuisance' is typically used to describe unwanted but generally un-harmful pollutants such as odour and noise (Environment Protection Act, 1990). Contaminants have been defined as substances which are naturally absent from the air or present in the air in an abnormally high concentration, and are potentially harmful (Safe Work Australia, 2011). Although bioaerosols could be, and have been previously described as a pollutants, contaminants and nuisances, throughout this thesis, bioaerosols will be referred to as pollutants, based on the serious negative health effects that bioaerosols could cause, as discussed in section 2.3.1,

2.3.3 Bioaerosol monitoring methods

The AfOR standardised protocol recommends that Andersen direct impaction samplers or IOM filter samplers should be used when monitoring bioaerosol concentrations at open windrow composting facilities (AfOR, 2009). Although not currently recommended in the AfOR protocol, liquid impingement methods have also been used extensively to monitor bioaerosols in numerous environments (Awad, 2007; Heinonen-Tanski *et al.,* 2009; Griffin *et al.,* 2011; Xia *et al.,* 2013). New and existing methods are also being continually developed and tested, including real-time measurement techniques (Jung *et al.,* 2012; Le Goff *et al.,* 2012; Su *et al.,* 2012; Beltelli, *et al.,* 2013). For example, Aerosol Fluorescence Sensors [AFSs] are being developed, which uses Ultra Violet [UV] light to target the fluorescence's of common amino acids found in

biological matter (Jung *et al.,* 2012). This section briefly reviews and critically assesses the widely used direct impaction, liquid impingement and filter sampling methods. Reviews comparing and critically assessing these and further monitoring techniques are available (Henningson and Ahlberg, 1994; Environment Agency, 2009b; Pankhurst, 2010).

The methods described below are mainly used to measure viable microorganisms, quantified in CFU/m^3 (Organics Recycling, 2009). However these methods may also be adapted to identify any non-viable and viable-but-non-culturable microorganisms present in the sample, through techniques such as microscopic analysis (Tamer Vestlund, 2009). This section reviews the use of these methods in the context of measuring viable microorganisms, as this is considered most frequently when collecting bioaerosols emitted from open windrow composting facilities. Therefore, the majority of existing datasets of bioaerosol concentrations measured at open windrow composting facilities have been collected using viable methods.

Direct Impaction

Direct sampling involves the pumping of the contaminated air across agar plates. The agar plates are filled with a selective medium, allowing the selected impacted bioaerosols to grow once incubated. It has been reported that the stress caused to the micro-organisms on impaction may result in loss of viability (Stewart et al., 1995; Environment Agency, 2009b). Direct impaction sampling using Andersen samplers are recommended in the AfOR sampling protocol (2009) for monitoring bioaerosols at composting facilities. Andersen samplers are produced from mainly metal materials (Thermo Scientific, 2013). This causes the device to be heavy, making it difficult to transport and use on site (Metha *et al.,* 1996). However, this also makes the sampler sturdy and unlikely to break. Agar plates are placed directly into the sampler to allow bioaerosols to be collected directly onto the surface of the agar, minimising post-processing work (Crook and Lacey, 1988; Li and Lin, 1999; Nesa *et al.,* 2001) as illustrated in Figure 2-2. This is advantageous as it potentially reduces overall sampling costs (Environment Agency, 2009b). Sampling costs may also be reduced as

the sampler can be used several times in one sampling trip. The sampler can be cleaned with ethanol between sampling runs, and agar plates can be replaced (Environment Agency, 2009b). Andersen samplers operate at a flow rate of 28.3 L/min (AfOR, 2009). This, and the fact that bioaerosols are impacted directly onto the media allow low concentrations of bioaerosols to be detected (Environment Agency, 2009b). This is particularly advantageous when measuring bioaerosol concentrations at, or close to, background levels. However this also makes it possible for the agar plates to become overloaded with bioaerosols, and thus impossible to count the number of colonies present after incubation (Environment Agency, 2009b). Therefore impaction samplers are unsuitable for use in areas where there are high concentrations of bioaerosols, for example close to the source of emissions (Eduard and Heederik, 1998).

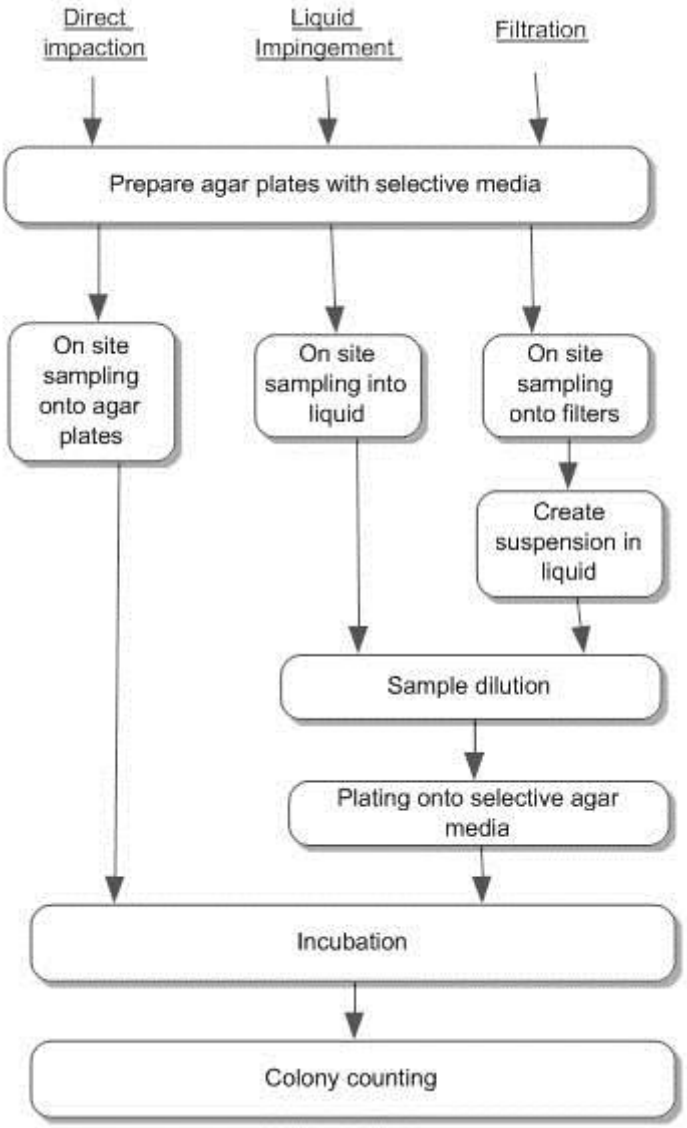

Figure 2-2 Flow diagram to illustrate the sampling processing procedures required to measure viable microorganisms for: Direct impaction, liquid impingement, and filtration sampling methods. Adapted from Drew *et al.* (2009)

Liquid Impingement

Liquid impingement is very similar to the impaction method, but instead of bioaerosols being impacted onto a solid agar surface, they are collected into a liquid. Sample post-processing is slightly more labour intensive than impaction sampling, as the liquid sample needs to be transferred to the selective media before incubation, as illustrated in Figure 2-2. If large concentrations of bioaerosol are expected, the liquid may also be diluted prior to transferral onto

agar plates. As the samples are collected into a liquid medium, there is also scope for multiple analyses from a single sample (Environment Agency, 2009b). Overloading is also less likely when compared to impaction sampling, and thus samplers can be run for extended time periods. However there is a risk of liquid loss through evaporation (Henningson and Ahlberg, 1994). It has also been reported that liquid mediums may not be suitable to collect fungal micro-organisms (Environment Agency, 2009b). Most liquid impingers, such as the AGI-30, are made from glass (Environment Agency, 2009b); part-plastic, part-metal versions, such as the Coriolis® are also available (Coriolis®, 2013). Glass impingers are light, compact and easily transportable, but are also fragile, and thus prone to breaking in the field, and operate at relatively low flow rates of 12.5 L/min (Environment Agency, 2009b; SKC, 2013). Coriolis®-style impingers are heavier, less transportable and more expensive but are less fragile, and can operate at high flow rates of 100-600 L/min depending on the model used (Coriolis®, 2013). Glass impingers require sterilisation before each use, therefore unlike Andersen samplers, a single glass impinger cannot be used more than once per sampling visit, which may increase overall running costs (Environment Agency, 2009b). Coriolis®-style impingers can be used more than once per sampling visit, but require replacement sterile sample collectors (Coriolis, 2013). To reiterate, liquid impingement methods are not currently recommended in the AfOR sampling protocol (AfOR, 2009).

Filtration

Filtration sampling involves air being passed through a filter using a pump. Any bioaerosols present in the air will be captured onto the filter. This method requires the most post-processing, as illustrated in Figure 2-2. Filters are transferred to a sterile liquid to allow the bioaerosols to be ‘washed’ from the filter and transferred onto selective agar. The agar is then incubated to allow growth. Similarly to liquid impingers, there is scope for multiple analyses from a single sample. IOM filter sampling heads are recommended in the AfOR protocol (AfOR, 2009), although other variations of filter sampler are available (BSI, 2011). IOM filter sampling heads are made mainly from plastic, making

them light, compact and easy to transport, like glass liquid impingers. Unlike glass liquid impingers, the plastic material causes them to be robust and less prone to breaking. Similarly to Andersen samplers, an IOM sampling head can be used several times in one sampling visit, providing that it is cleaned with ethanol, although fresh filters and cassettes are still required. IOM filtration samplers are used at a low flow rate, 2L/min (AfOR, 2009) and thus have a high LLOD (Pankhurst, 2010). Despite having a high LLOD, IOM filtration samplers may still get overloaded with micro-organisms (Eduard and Heederik, 1998). It should be noted that filtration methods using higher flow rates (50L/min) are available (BSI, 2011), thus lowering LLOD levels. Similarly to liquid impingers, filtration samplers can be used for extended time periods. However it has been reported that some viability may be lost when using IOM samplers for longer than thirty minutes, particularly for bacterial cells (Wang *et al.,* 2001). However due to their robustness, compactness and because they are light, this sampling technique is more suited to areas where high concentrations of micro-organisms are likely, such as in areas close to the source of pollutant emission.

2.3.4 An overview of bioaerosol monitoring data collected at open windrow composting facilities

Many monitoring methods, including those described in section 2.3.3, have been used to collect bioaerosols downwind of open windrow composting facilities, during agitation activities (Weber *et al.,* 1993; Danneberg *et al.,* 2007; Lacey, 1997; Fischer *et al.,* 1999; Wheeler *et al.,* 2001; Taha *et al.,* 2006; SNIFFER. 2007; HSE, 2010; Pankhurst *et al.,* 2011). Although there are many studies that have reported bioaerosol measurements downwind of open windrow composting facilities during agitation activities (Weber *et al.,* 1993; Fischer *et al.,* 1999; Wheeler *et al.,* 2001; Sanchez-Monedero and Stentiford, 2003; Taha and Pollard, 2004; SWICEB, 2005; Taha *et al.,* 2006; SNIFFER. 2007; Taha *et al.,* 2007; HSE, 2010), there has been a lack of a detailed, extensive, and consistent measurement database, of bioaerosol concentrations collected in these conditions. For example, data has been collected:

- Using different monitoring techniques
- In different locations
- By different sampling teams
- Over very short time scales
- Enumerating different bioaerosol components

This has provided snapshots of bioaerosol emissions spatially and temporally. However it is important to consider the fact that collecting data is very time consuming and expensive (Pankhurst, 2010). These factors combined has meant that the performance of dispersion models in the open windrow composting context has not been fully evaluated, as there has been a lack of a consistent, extensive measured dataset to compare modelled outputs to. Testing modelling performance is paramount, as models have the potential to provide a more continual overview of emissions in space and time, in different operating and metrological conditions. If modelled outputs were reliable, then dispersion models could be used to enhance the understanding of exposure to nearby sensitive receptors, and thus improve the knowledge of the levels of exposure required to lead to the onset of negative health issues. They could also be used to predict bioaerosol emissions from facilities that wish to expand, or do not yet exist.

Recently, an unpublished full comprehensive database became available (Pankhurst, 2010). Pankhurst successfully completed the project aim of providing a “reliable, validated data-set describing the emission and dispersal of bioaerosols from composting facilities” (Pankhurst, 2010). This was achieved by quantitatively characterising bioaerosol emissions emitted during agitation activities on open windrow composting facilities, up to and beyond 250 metres of the composting site boundary. Bioaerosols were collected using consistent methods in the field and the laboratory, and all samples were replicated. Data was collected at two different composting facilities, over the course of a year, thus capturing bioaerosol concentrations in varying seasonal and meteorological conditions. Therefore model performance in this specific context

can be tested using these datasets. Dispersion models are described and discussed in section 2.4.

2.4 Introduction to dispersion modelling

An air dispersion model is a mathematical simulation that uses equations of atmospheric airflow to simulate how air pollutants disperse (Chang and Hanna, 2004), by describing the atmosphere, dispersion, and physical and chemical processes within the plume to calculate concentrations at various locations (Holmes and Morawska, 2006). Dispersion models require certain input parameters, principally meteorological and emissions data (Kuhlwein and Friedrich, 2000; Gostelow *et al.,* 2004; Sharma *et al.,* 2004; Kesarkar *et al.,* 2007). Emissions data has been difficult to measure in the open windrow composting scenario. This has been due to the fact that bioaerosol emissions are difficult to measure and capture because:

- Emissions are not controlled or contained
- Bioaerosols are emitted continuously, in different quantities. Higher concentrations are associated during agitation activities (Taha *et al.,* 2006)
- Open windrow composting facilities are dangerous environments to sample in (Taha *et al.,* 2006)

Pollutant dispersal is controlled primarily by atmospheric turbulent fluctuations (Simms et al., 2000; Chang and Hanna, 2004; Sheridan et al., 2004).Turbulence is random by nature, and thus cannot be precisely predicted by air dispersion models (Chang and Hanna, 2004). Despite model advancements and increasing model complexity, no dispersion model can provide a perfect prediction of observed conditions (Holmes and Morawska, 2006), only a simple simulation of what occurs in nature (McIntyre, 2000; Chang and Hanna, 2004). There are also uncertainties in model physics, which can lead to input data errors (McIntyre, 2000; Chang and Hanna, 2004).

2.4.1 Regulation

Currently, there is no regulation regarding what dispersion model should be used when modelling bioaerosol emissions from composting facilities (Environment Agency, 2000). The Royal Meteorological Society has published guidance for the preparation of dispersion modelling assessments (Ireland *et al.,* 2004) and states that the model chosen should adequately describe the circumstances being assessed, and that outputs should be sufficient for assessment. The Environment Agency also recommends that the choice of model should be justified and described (Environment Agency 2000; 2010). Additionally, the Ministry for the Environment in New Zealand (Bluett *et al.,* 2004) recommend that an appropriate model should be chosen based on the complexity of the dispersion and the significance of potential effects (Bluett *et al.,* 2004).Types of dispersion model

There are many types of dispersion model including: Box, Gaussian, Langrangian, Eulerian, and Computational Fluid Dynamics [CFD] (Sharma *et al.,* 2004; Holmes and Morawska, 2006; Gorlé *et al.,* 2009). Each type of dispersion model is summarised in Table 2-4 and reviewed below. Dense gas models are also available, which simulate the dispersion of pollutants denser than air. This type of model has not been summarised or reviewed, as there is currently no evidence to suggest that bioaerosols are denser than air. However, bioaerosols are expected to settle due to gravitational effects, but this can be simulated within other model types.

Table 2-4 Brief definitions of the most commonly used types of atmospheric dispersion model (Haug 1993; Turner, 1994; Barratt, 2001; Hanna *et al,.* 2004; Holmes and Morawska, 2006; Gorlé *et al.,* 2009; Acero *et al.,* 2012; Wen *et al.,* 2012)

Model Type	Brief Description
Box	Simplest type of model. Assumes that the given volume of atmospheric air in a region or site is the shape of a box and that the pollutants inside the box are homogeneously distributed.
Gaussian	Assumes that the air pollutant has Gaussian distribution (i.e. the pollutant distribution has a normal probability distribution) horizontally and vertically. Gaussian models can predict the dispersion of continuous or non-continuous (puff) emissions, originating from low or elevated heights.
Lagrangian	Similar to box models because they define a region of air as a box containing an initial concentration of pollutants. The model mathematically follows the course taken by the box as it moves downwind (referred to as a 'random walk process'). Uses a moving frame of reference as the boxes move from their initial location
Eulerian	Similar to a Lagrangian model, but the main difference is that it uses a fixed three dimensional Cartesian grid as a frame of reference instead of a moving reference.
Computational Flow Dynamics [CFD]	Provides a complex analysis of fluid flow based on conserving mass and momentum by resolving the Navier-Stokes equation and by using a small grid size.

Box models

Holmes and Morawska (2006) stated that box models do not provide any information on local pollutant concentrations, where concentrations are influenced by local changes to wind and emissions. Therefore box models are inappropriate when modelling bioaerosol emissions from composting facilities. This is because, due to current recommendations, researchers and regulatory bodies are interested in bioaerosol concentrations within the first 250 metres of dispersion.

CFD, Eulerian and Lagrangian models

Lagrangian and Eulerian models are increasingly being used to simulate highly complex and non-linear photochemical reactions (Sharma *et al.,* 2004; Vautarrd *et al.,* 2007; Wols and Hofman-Caris, 2012). CFD models can simulate gas dispersion in more geometrically complex situations, providing outputs of flow fields, turbulence levels and concentration fields, and can predict dispersal around buildings (Riddle *et al.,* 2004; Maïzi *et al.,* 2010). As a result of this, they are increasingly being used to simulate pollutant dispersion in urban areas (Hanna *et al.,* 2004; Sharma *et al.,* 2004; Hang *et al.,* 2009; Acero *et al.,* 2012). CFD, Eulerian and Lagrangian models cannot be conveniently used, especially for regulatory purposes due to the thorough mathematical computations, large input data and larger computational capabilities required (Govaerts, 1989; Lines *et al.,* 1997; Ormerod, 2001; Riddle *et al.,* 2004; Sharma *et al.,* 2004; Schatzmann and Leitl, 2011). CFD models have also been found to run slowly (Hanna *et al.,* 2002), under predict measured concentrations by 20% (Hanna *et al.,* 2004) and they do not account for meandering wind conditions (Riddle *et al.,* 2004). Due to the complicated nature of these types of model, they will not be used in this study.

Gaussian models

Gaussian models have found favour in the scientific community (Sharma *et al.,* 2004), particularly when modelling odour emissions (McIntyre, 2000; Witherspoon *et al.,* 2000; Sarkar *et al.,* 2003; Sironi *et al.,* 2003; Dincer *et al.,* 2004; Gostelow *et al.,* 2004; Sheridan *et al.,* 2004; Hayes *et al.,* 2006; Latos *et al.,* 2011; Vieira de Melo *et al.,* 2012), and have also been the model of choice thus far when simulating bioaerosol dispersion from composting facilities (Millner *et al.,* 1980; Dowd *et al.,* 2000; Taha and Pollard, 2004; Taha *et al.,* 2004; 2005; 2006; 2007; ADAS, 2005; Drew *et al.,* 2005; 2007; SNIFFER 2007). Basic Gaussian plume models assume that there are no interactions between multiple pollutant plumes, and cannot model the recirculation effects caused by the presence of buildings, (Holmes and Morawska, 2006). Furthermore, some Gaussian models cannot accurately estimate pollutant

concentrations in very low wind speeds (Sharma, *et al.,* 2004; Qian and Venkatram, 2011). However, 'new generation' Gaussian models are now available, which use improved methods to describe diffusion and dispersion in the atmosphere (Bluett, *et al.,* 2004). This has allowed the effects of buildings, low wind speed and complex terrain to be modelled (Bluett *et al.,* 2004; Carruthers *et al.,* 2009; Wanger and Dubbs, 2011). Gaussian models are relatively more accurate and consistent with the random nature of atmospheric turbulence, and are considered to be best suited for pollutant dispersion (Sharma *et al.,* 2004). From the information reported above, Gaussian models appear to be the most suitable type of dispersion model to use when modelling bioaerosol emissions, and thus will be used in this study.

2.4.2 Gaussian models

In statistics, the Gaussian distribution is a bell-shaped distribution which is used to approximate any variable that tends to cluster around the mean (Beychok, 1994; Wheater and Cook, 2006). Gaussian plume models assume that pollutant emissions are normally distributed, horizontally and vertically (Lines *et al.,* 1997; Mussio *et al.,* 2001). This has the effect of producing a plume of polluted air that is approximately cone-shaped, with the apex of the cone towards the source of the emission (Smith, 1995; Sheridan *et al.,* 2004). This is illustrated in Figure 2-3 and described mathematically in Equation 2-1.

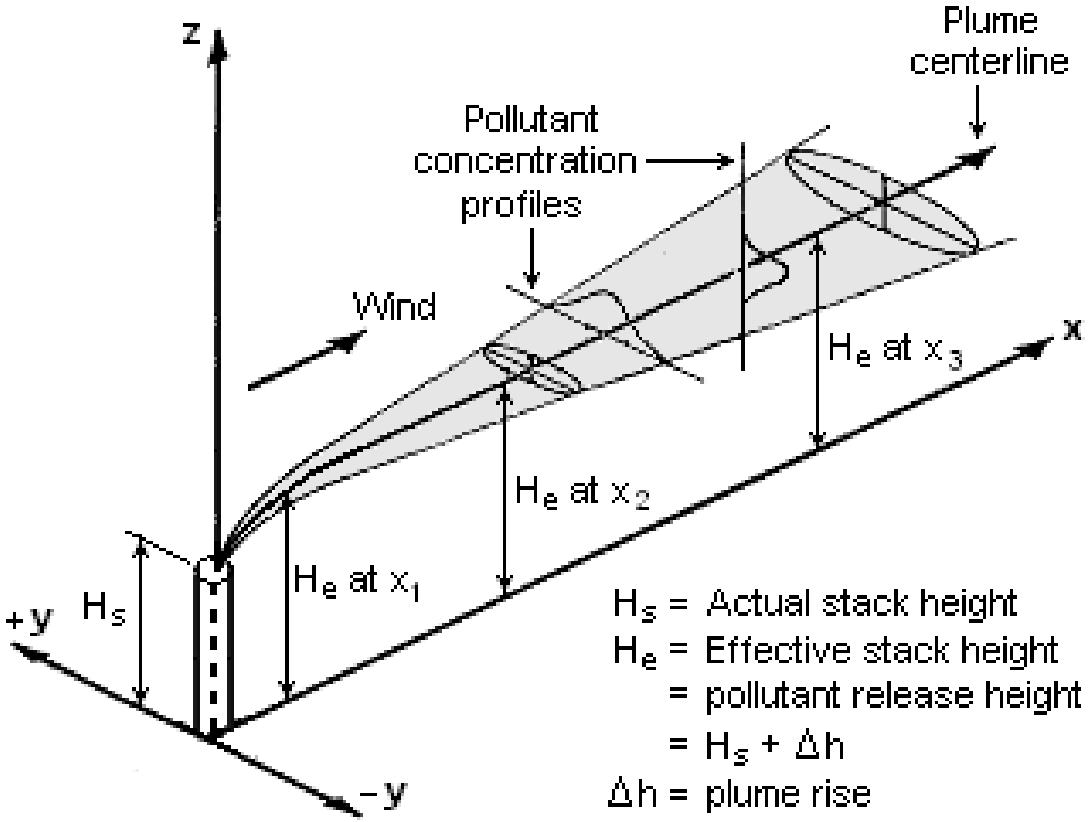

Figure 2-3 A typical visualisation of a buoyant Gaussian pollutant dispersion plume from a point source (Beychok, 2007)

Figure 2-3 shows that as the plume moves away from the source, the pollutants in the plume become more diluted as the plume expands laterally and vertically due to the effects of turbulence.

$$\chi_{(x,y,z,H)} = \frac{Q}{2\pi\sigma_y\sigma_z U}\exp\left[\left(\frac{-y}{2\sigma_y}\right)^2\right]\left\{exp\left[-\frac{(z-H)}{2\sigma_z}\right]^2 + exp\left[-\frac{(z+H)}{2\sigma_z}\right]^2\right\}$$

Equation 2-1

Where:

χ is the pollutant concentration at point (x, y, z, H) (g/m^3)

x Is the downwind distance from the source (m)

y is the lateral distance from the source (m)

z is the vertical distance above the ground (m)

H is the effective source height above the ground (m)

Q is the pollutant emission rate (g/s)

σ_z is the plume dispersion parameter in the vertical direction (m)

σ_y is the plume dispersion parameter in the horizontal direction (m)

U is the wind speed (m/s)

(Keddie, 1980; Essa *et al.,* 2003)

2.4.3 Types of Gaussian model

There are many Gaussian models available, each having different advantages and disadvantages. Table 2-5 briefly describes the most commonly used Gaussian air dispersion models, and outlines the main advantages and disadvantages of each.

Table 2-5 A brief summary of the advantages and disadvantages of each of the most commonly used Gaussian dispersion models

Gaussian air dispersion model	Model description	Advantages	Disadvantages
ADMS	Atmospheric Dispersion Modelling System [ADMS] is an advanced steady state 'new generation' dispersion model (Hanna *et al.,* 2000; Sharma *et al.,* 2004; CERC, 2010b). Horizontally and vertically, the plume concentration distribution in ADMS is Gaussian during neutral and stable conditions. During unstable conditions the vertical plume concentration distribution is non-Gaussian (Riddle *et al.,* 2004). ADMS uses current understanding of the structure of the atmospheric boundary layer, describing it using the Monin-Obukhov length (Carruthers *et al.,* 1994; McHugh *et al.,* 1999; Riddle *et al.,* 2004).	Can be applied to point, line, area, volume and jet sources, (Hanna *et al.,* 2000) Able to model complex terrain and building effects (Simms *et al.,* 2000), short duration releases (Taha *et al.,* 2007), pollutant removal due to wet and dry deposition, coastal effects and chemical effects (CERC, 2010) Uses current understanding of the structure of the atmospheric boundary layer (Riddle *et al.,* 2004: Sheridan *et al.* 2004). In an evaluation between the ADMS, AERMOD and ISC models, ADMS was suggested to perform the best (Hanna *et al.,* 2000)	Unable to model very low wind speeds <0.1m/s (CERC, 2010) The wind flow model, FLOWSTAR which is incorporated into ADMS, is a linear model, which is constrained due to the simplifications in its calculations (Hall *et al.,* 2000a) Modelling emissions near to the equator or the pole may lead to significant errors in the calculation of the boundary layer parameters (CERC, 2010)

Gaussian air dispersion model	Model description	Advantages	Disadvantages
CALPUFF	California Puff Model [CALPUFF] is a time and space dependent Gaussian dispersion model (Sironi *et al.,* 2003), used to simulate non-steady state dispersal (Dionne, 2011). CALPUFF was originally developed by the Sigma Research Corporation under sponsorship from the California Air Resources Board (Scire *et al.,* 1990). Ownership now belongs to TRC Environmental Corporation (TRC, 2012). It can be used to model pollutant dispersal within tens of metres of the source to hundreds of kilometres (US EPA, 2012b). CALPUFF is able to treat differing meteorological effects in time and space on pollutant transport and dispersion (US EPA, 2012b)	Can be used to model point, area, volume and line sources (US EPA, 2012b) Capable of modelling the effects of buildings, complex terrain, wet and dry deposition and coastal effects (US EPA, 2012b)	Tends to under-predict mean and maximum concentrations (Holmes and Morawska, 2006) More complex than AERMOD and thus requires more data, modelling decisions, and calculation times (Dionne, 2011) May provide a less accurate estimation of emissions within short distances of the source, (Hoffnagle, 2008; Dionne, 2011) Unable to simulate building effects when modelling as an area or volume source (Ministry for the Environment, 2004)

Gaussian air dispersion model	Model description	Advantages	Disadvantages
AERMOD	AERMOD is a 'new generation' steady state Gaussian model (Ministry for the environment, 2004; Sharma *et al.,* 2004). It was developed by the AMS/EPA Regulatory Model Improvement Committee [AERMIC] as an intention to replace the ISC3 model prescribed by the US EPA (Hanna *et al.,* 2000). Like ADMS, AERMOD describes the atmospheric boundary in terms of the Monin-Obukhov length (McHugh *et al.,* 1999), and dispersion in unstable conditions is non-Gaussian (Ministry for the Environment, 2004). It also uses a modified Briggs formula to calculate plume variables (McHugh *et al.,* 1999).	Can model multiple source types including point, area and volume sources Capable of modelling the effects of buildings (Perry *et al.,* 2004), complex terrain (Cimorelli *et al.,* 2004), and wet and dry deposition (US EPA 2012a) Can estimate particle deposition using a crude reflection coefficient algorithm. Can also model the effects of complex terrain (Ministry for the Environment, 2004) Dispersion from different release heights is better, as turbulence simulations can vary with height Ministry for the Environment, 2004)	Requires thorough meteorological input values, and a lot of data preparation prior to running (Vallamsundar and Lin, 2011) Assumes constant meteorological conditions (Perry *et al.,* 2004)

Gaussian air dispersion model	Model description	Advantages	Disadvantages
ISC/ISCST3	Industrial Source Complex model [ISC] is a straight line trajectory Gaussian model, which uses Pasquill/Gifford atmospheric stability classes to describe turbulence in the boundary layer (Hall and Spanton, 1999). The model comes in two forms; one for calculating long-term average concentrations and another for short-term average concentrations (US EPA, 1995a). The short-term version of the model is often referred to as the Industrial Source Complex Short Term model or ISCST. The model also has a screening version, called SCREEN (Lakes Environmental, 2012b)	Point, area and volume sources can be modelled Capable of modelling the effects of wet and dry deposition (US EPA, 1995a; Ministry for the Environment, 2004) Easy to use, as it can be used with minimal meteorological inputs (Hanna *et al.,* 2000)	Not suitable for modelling the effects of buildings (Simms *et al.,* 2000) or complex terrain (Ministry for the environment, 2004), Can be unreliable due to its simplicity (Ormerod, 2001) Tends to perform more poorly when compared to AERMOD and ADMS (Hanna *et al.,* 2000) Uses outdated stability classes (Hall and Spanton, 1999) and does not incorporate advanced understanding of turbulent processes in the boundary layer (Hanna *et al.,* 2000)

Gaussian air dispersion model	Model description	Advantages	Disadvantages
AUSPLUME	AUSPLUME is a steady-state Gaussian model, available to purchase from the Environment Protection Authority [EPA], Victoria, Australia, (Ministry for the Environment, 2004). The model uses the outdated horizontal dispersion coefficients, Pasquill-Gifford, Briggs Rural and Sigma Theta (Ministry for the Environment, 2004). It also assumes that meteorological conditions are constant (Ministry for the Environment, 2004).	Can model point, area and volume sources Able to model the effects of buildings (Ministry for the Environment, 2004) Suitable for use in near-field applications (Ministry for the Environment, 2004) Can estimate particle deposition using a crude reflection coefficient algorithm. Is capable of modelling the effects of complex terrain for selected source types (Ministry for the Environment, 2004)	Unable to model the effects of complex terrain for every source type (Ministry for the Environment, 2004) Unable to model the effects of buildings when modelling as an area or volume source (Ministry for the Environment, 2004) Assumes constant meteorological conditions (Ministry for the Environment, 2004) Cannot calculate thermal buoyancy effects when modelling as an area source (Ministry for the Environment, 2004) Uses outdated horizontal dispersion coefficients (Ministry for the Environment, 2004)

2.5 Dispersion modelling of bioaerosols from composting facilities

Several bioaerosol components have been modelled in a number of different environments. For example, the dispersion of *Legionella* species from cooling towers (Ulleryd *et al.,* 2012) has been modelled, as well as the dispersion of *Coxiella* from sheep farms (Wallensten *et al.,* 2010). Ulleryd *et al.* (2012) studied an outbreak of Legionnaire's Disease after the number of pneumonia cases reported at the local hospital increased. *Legionella pneumophila* species, the agent of Legionnaire's disease, were detected in samples from cooling towers. Modelling was used to simulate the probable spread from these cooling towers. This study identified that modelling provided a useful tool when investigating epidemiological outbreaks of a bioaerosol-related health problems, in other words, emergency outbreaks. Similarly, Wallensten *et al.* (2010) studied the causes of an outbreak of Q fever, which is caused by *Coxiella burnetii.* Wallensten *et al.* (2010) hypothesised that the outbreak was caused by three high risk sheep farms. Modelling was used to assess whether it was possible that *Coxiella burnetii* emissions from these farms could have travelled into the nearby town, thus causing the onset of the reported cases of Q fever. Using a dispersion model supported the hypothesis that the farms had caused the unexpected outbreak in Q fever. The purpose of dispersion modelling within these studies was to apportion a source to a particular pollutant problem, not to accurately predict bioaerosol concentrations from a source at a particular location. Therefore, the way in which the dispersion model was used by Ulleryd *et al.* (2012) and Wallensten *et al.* (2010) is not suitable for the purpose of this study, to estimate bioaerosol concentrations downwind of an open windrow composting facility. Additionally, as the relationship between bioaerosols released from open windrow composting processes and negative health effects has not yet been fully established.This type of modelling is not yet useful in the open windrow composting scenario. Moreover, bioaerosol emissions from open windrow composting processes are continuous non-emergency releases, which are highly variable over time, dependant on site conditions. Successful

modelling of bioaerosols from the open windrow composting process needs to be established to help identify the relationship between exposure levels and the onset of negative health impacts. However, there are only a limited number of studies that have used dispersion models to estimate the concentration of bioaerosols emitted from composting facilities. Ten studies modelled bioaerosol dispersion from open windrow composting facilities (Environment Agency, 2001b; Taha and Pollard, 2004; ADAS, 2005; Taha *et al.,* 2004; 2005; 2006; Drew *et al.,* 2005; 2007; SNIFFER, 2007; Tamer Vestlund, 2009), and of these ten studies, seven modelled bioaerosol dispersion from agitation activities (Environment Agency, 2001b; Taha and Pollard, 2004; ADAS, 2005; Taha *et al.,* 2006; Drew *et al.,* 2007; SNIFFER, 2007; Tamer Vestlund, 2009). There are no known journal articles, conference papers or other publications of modelling studies of bioaerosol emissions from composting facilities since 2009 (the study by Tamer Vestlund (2009) is reported within an unpublished PhD thesis). All studies which have modelled bioaerosol dispersion from composting facilities are reviewed in Table 2-6, to highlight:

- The lack of statement of what input parameter values were used within the dispersion models used in the studies
- The large variability of the input values used for some of the parameters
- The lack of justification of why certain values have been used as inputs to the dispersion model

Table 2-6 Details of the model and model inputs used in the studies that have attempted to model bioaerosol emissions from composting facilities. NS indicates that the information has not been stated. All figures are stated to one decimal place. Some values have been converted to correspond to SI standards

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	Pollutant emission rate(s) (units)	Geometry of the emission source (units)	Wind speed (m/s)	
Millner *et al.,* (1980)	Model of Pasquill	Windrow drying, turning, screening, vehicle movements	Point	$2.3x10^{4}$ – $6.7x10^{10}$ (particles per second)	Height 5.0m	2.1 – 3.6	Agitation activities modelled as sources Receptor height was 2.1m Emission rate calculated by solving the equation, using the aid of the model with Gifford conversion

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	Pollutant emission rate(s) (units)	Geometry of the emission source (units)	Wind speed (m/s)	
Danneberg *et al.,* (1997)	AUSTAL-PC 3.2	Screening	Point	$1.3x10^{7}$ -$2.8x10^{8}$ (CFU/s) for Total Bacteria $4.6x10^{6}$ (CFU/s) for *Aspergillus fumigatus*	NS	NS	Emission rate was calculated using measured concentrations at 150 metres downwind, and measurements made 'near to a rotating sieve', assumes to be a screener, by means of recalculation in the model and by the use of Giebel's formula, which was multiplied by a factor of 2 to account for low emission height

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	Pollutant emission rate(s) (units)	Geometry of the emission source (units)	Wind speed (m/s)	
Dowd *et al.,* (2000)	Original and modified point source model and an area model	NS	Point and Area*	Point: $2.0x10^6$ and $2.7x10^1$ (organisms per second) for Salmonella and coxsackievirus respectively Area: $5.1x10^6$ and $7.5x10^2$ (organisms/m^2/s)* for Salmonella and coxsackievirus respectively	Height 2.0m	2.2 (mean), and less than 8.9	Emission rate estimated via back calculations using actual sampling data

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	Pollutant emission rate(s) (units)	Geometry of the emission source (units)	Wind speed (m/s)	
Environ-ment Agency (2001b)	SCREEN 3	Screening, turning and shredding, for two open windrow sites, and feed processing and unloading for in-vessel	NS	NS	NS	NS	Used results from filter samplers only Used one-hour averages Source height and emission rate adjusted until a good fit with the measured data was achieved
Taha and Pollard (2004)	SCREEN 3	Turning and 'agitation'	Point	$2.4x10^8$ – $8.9x10^8$ and $4.8x10^8$ – $8.6x10^8$ (CFU/s) For *Aspergillus fumigatus* and actinomycetes respectively	Height 0 metres Diameter 3 metres	0.1	Temperature of 11ºC was also inputted Emission rates were back calculated

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	Pollutant emission rate(s) (units)	Geometry of the emission source (units)	Wind speed (m/s)	
ADAS (2005)	ADMS	'Activities'	Area	$6.0x10^{-6}$ ($g/m^2/s$)	Height 1.0 - 1.8 metres Areas 2.0 by10.0 metres and 2.0 by1.0 metres	3.1-3.3	Roughness length 0.2 metres Emission rates determined by scaling model outputs to match the measured data
Taha *et al* (2004; 2005)	SCREEN 3	No agitation activities monitored, only static compost windrows	Area	$3.6x10^3$ – $1.1x10^4$ and $5.5x10^3$ – $2.2x10^4$ ($CFU/m^2/s$) for *Aspergillus fumigatus* and actinomycetes respectively	Height 2 metres Area 20 by 80 metres	NS	Emission rate calculated using an adapted odour emission rate equation (Jiang and Kaye, 2001)

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	Pollutant emission rate(s) (units)	Geometry of the emission source (units)	Wind speed (m/s)	
Drew *et al.,* (2005)	ADMS 3.3	As per Taha *et al.,* (2005)	Point	$8.3x10^3$ ($CFU/m^2/s$) assumed to have been adapted to enable modelling of a point source	Height 1.8 metres Diameter of 1.0 metre	NS	Used data from Taha *et al.,* (2005) Source temperature of 17.5ºC was modelled; this was the measured ambient temperature on the day of sampling. Exit velocity of 0.19m/s was also modelled

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	**Pollutant emission rate(s) (units)**	**Geometry of the emission source (units)**	**Wind speed (m/s)**	
Taha *et al.,* (2006)	SCREEN 3	Static emissions were monitored as well as screening, turning and loading operations	Point, and Area	Static emission, $8.8x10^3$ CFU/m^2/s for *Aspergillus fumigatus* Agitation activities, point sources stated only $2.0x10^5$ – $8.9x10^8$ and $7.0x10^5$ – $8.6x10^8$ (CFU/s) for *Aspergillus fumigatus* and actinomycetes respectively	Static emissions, height 1.5 to 2.0 metres Agitation activities height 0 metres and 3 metres diameter for point source	0.6-3.9m/s	Emission rate calculated using an adapted odour emission rate equation (Jiang and Kaye, 2001) for static emissions For agitation activities, the emission rate was back calculated, estimated by using multiple candidate emission rates until the model outputs resembled measured data Measured ambient temperatures of 16.3-19.3ºC A source temperature of 11.0º was inputted into the model

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	Pollutant emission rate(s) (units)	Geometry of the emission source (units)	Wind speed (m/s)	
Drew *et al.,* (2007)	ADMS 3.3	Static emissions were monitored as well as shredding, turning and screening activities	Point and Area*	Static emissions 0.0-1.6x10^5 and 8.0x10^4-3.6x10^5 (CFU/m^2/s)* for *Aspergillus fumigatus* and actinomycetes respectively Agitation activities, 1.8x10^4 – 1.6x10^5 and 7.9x10^3 – 3.6x10^5 (CFU/s) for *Aspergillus fumigatus* and actinomycetes respectively	Static as 4 point sources each with a diameter of 20 metres	NS	For summer emissions, a source temperature of 30ºC was used whereas a source temperature of 15ºC was used during winter emissions

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	Pollutant emission rate(s) (units)	Geometry of the emission source (units)	Wind speed (m/s)	
Taha *et al.,* (2007)	SCREEN 3 and ADMS 3.3	Static emissions modelled as well as Screening, turning and loading activities	Point and Area	Agitation activities $5.5x10^2$ – $1.6x10^4$ and $4.8x10^2$ – $1.1x10^4$ (CFU/s) for *Aspergillus fumigatus* and actinomycetes respectively	Static as area source 80 by 20 metres Agitation activities as a point source with a diameter of 3 metres Source release height of 3 metres and 2 metres for agitation activities and static emissions respectively.	NS	Emission rate calculated using an adapted odour emission rate equation (Jiang and Kaye, 2001) for static emissions Agitation activity emission rates were calculated by back extrapolation of the measured data. An exit velocity of 0.2 and 0.3 metres per second[#] was used for agitation activities and static emissions respectively A source temperature of 9.9°C or 15.0°C was used Modelled using stability class D Roughness length of 'rural' and 0.1 metres was used in the SCREEN3 and ADMS 3.3 models respectively

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	Pollutant emission rate(s) (units)	Geometry of the emission source (units)	Wind speed (m/s)	
SNIFFER (2007)	SCREEN 3 and ADMS 3.3	Passive emissions and turning, shredding and screening agitation activities	Point, Area and Volume	Point sources: $2.0x10^{1}$ – $5.3x10^{5}$ and $1.2x10^{2}$ – $6.1x10^{6}$ (CFU/s) Area sources: $1.1x10^{2}$ – $1.2x10^{2}$ and $9.4x10^{1}$ – $2.5x10^{2}$ (CFU/m^{2}/s) Volume sources $5.9x10^{3}$ – $2.6x10^{7}$ and $2.7x10^{4}$ – $1.4x10^{8}$ (CFU/m^{3}/s)	NS	NS	Bioaerosol emission rate for passive emissions was estimated using adapted odour emission rate equations (Jiang and Kaye, 2001) Emission rates for agitation activities were estimated by back extrapolation Stability class D was modelled Building dimensions are stated

Reference	Dispersion model(s) used	Agitation activities modelled	Model inputs used				Other information or Model inputs
			Source type(s)	Pollutant emission rate(s) (units)	Geometry of the emission source (units)	Wind speed (m/s)	
Tamer Vestlund (2009)	ADMS 3.3	Passive emissions and agitation activities	Point and Area	$2.6x10^2$ – $6.4x10^3$ CFU/m^2/s for an area source and $5.8x10^7$ – $8.1x10^7$ CFU/s for an area source, for actinomycetes	All sources modelled at a height of 3 metres. Static as area source (size not stated) Agitation activities as a point source with a diameter of 3 metres	NS	Several pollutant temperatures were modelled, equating to ambient temperature (19.7-28.5°C) and a 'high temperature scenario' (55°C) Several exit velocities were used from 0.5 metres per second to 1.7m/s Stability class D was modelled

* Dowd *et al.* (2000) and Drew *et al.* (2007) state emission rates of units of organisms or CFU per second when modelling with an area source type. This is not the standard unit when modelling an area source, therefore a typographical error has been assumed, and this unit has been altered to the standard CFU or organisms/m^2/s
# Taha *et al.* (2007) states an exit velocity with units in m. As the standard unit for exit velocity is m/s, a typographical error has been assumed and thus has been altered as such within the table

The most striking features of the studies summarised in Table 2-6 are:

- The fact that many studies have not fully stated all of the input values used within the dispersion model
- Of those input values which have been disclosed, the majority have not been justified, and thus the detail of how these values have been measured or estimated is missing
- A large range of emission rates has been used within the dispersion model

An assessment of the model inputs used within the studies presented in Table 2-6 is presented in sections 2.5.1 to 2.5.5. Each input is described and critically assessed singularly.

As so many studies have not stated or justified the model inputs used within the dispersion models, this emphasises the fact that there is a lack of measurement data for many input parameters in the context of the open windrow composting scenario. It should be appreciated that collecting samples in the open windrow composting environment is very difficult, due to the dangers of working in this environment (Taha *et al.,* 2006) and the fact that emissions are not controlled, contained, or released in a continuous quantity (for example, agitation activities cause higher bioaerosol concentrations (Taha *et al.,* 2006)).

2.5.1 Pollutant emission rate

The pollutant emission rate is one of the most important model inputs, as it represents the amount, and rate of material emitted from the source of the release (Barratt, 2001). To reiterate, the emission rate, sometimes referred to as the mass flow rate (Mensink and Maes, 1997) is represented by the symbol ‘Q’ in Equation 2-1. Table 2-6 highlights that the emission rates used to model composting agitation activities vary by several orders of magnitude, depending on the source type modelled. The emission rates used were obtained by using bioaerosol measurements to calculate or back extrapolate an emission rate. The measurements used to estimate an emission rate were taken at various distances downwind of the source of the agitation activities, as outlined below:

- ‘As close as practically possible’ and 30 metres (Drew *et al.,* 2007)
- 2-10 metres (SNIFFER, 2007)
- 5 -10 metres (Taha *et al.,* 2006; Taha *et al.,* 2007)
- 10 metres (Taha and Pollard, 2004)
- 15 metres (Tamer Vestlund, 2009)
- 10-100 metres (Environment Agency, 2001)
- 150 metres (Danneberg *et al.,* 1997)
- Not detailed (Miller *et al.,* 1980)

Ideally, emission rate estimations would be based on measurements taken directly at the source of emission, not from concentrations taken from 2 metres or more from the source. This is because the pollutant plume begins to rise and disperse causing pollution concentrations to become diluted immediately upon release (Beychok, 1994). The rate of plume dispersal depends on many factors including: source geometry, pollutant temperature, pollutant exit velocity and meteorological conditions (Beychok, 1994). Hence emission rates have been based upon measurements that are not representative of true concentrations at source. It has not yet been possible to measure emissions directly at source during agitation activities, due to the dangers of working at composting facilities because:

- Heavy machinery with moving parts is used to agitate the compost
- There may be poor visibility due to emissions of steam and dust during agitations
- Noise levels are high due to the machinery used to agitate the compost

It is also physically difficult to place the samplers at the source of the agitation as some samplers can be heavy, and orientated in a specific direction. The samplers may also not be capable of capturing the whole of the release as plumes from agitation activities may originate from large areas, such as from the screening process, or the source of the agitation may move, for example when turning windrows.

Direct measurements have been possible when measuring emissions from static windrows by using a portable wind tunnel (Taha *et al.* 2005; 2006; 2007; Drew *et al.,* 2007; Tamer Vestlund, 2009). However this method is not practical for use during agitation activities (Taha *et al.,* 2006; 2007). Therefore two main methods have been used to estimate emission rates during agitation activities: calculation and back extrapolation, as reviewed individually below.

Emission rate calculation

Millner *et al.* (1980) and Danneberg *et al.* (1997) estimated emission rates by re-arranging model equations. Millner *et al.* (1980) rearranged the equation used by the model of Pasquill. A bioaerosol concentration collected from a specified point in time and space was inputted into the model, along with several other model inputs to calculate and emission rate. Danneberg *et al.* (1997) also utilised this method, using Giebel's formula. The emission rate calculated can be re-entered into the dispersion model to estimate emissions at locations where pollutant concentrations were not measured.

There are several limitations when using this method:

1. To be able to apply this method, the equations and algorithms used by the model must be known so that the equation can be re-arranged. Millner *et al.* (1980) used the very simple model of Pasquill, based on a single equation that can be rearranged with ease. More recent models use several equations of greater complexity, thus applying this method to these models would be extremely time consuming and impractical. Danneberg *et al.* (1997) used the even simpler Giebel's formula. These equations do not incorporate current knowledge of turbulence within the boundary layer or plume buoyancy effects.
2. When rearranging the equation to calculate an emission rate, all other equation inputs must be known, which may be difficult to measure. The number of additional inputs needed depends on the complexity of the model.
3. The emission rate calculated using this method will be based on a measurement sampled at a distance away from the source. Although this

distance is not stated in Millner *et al.* (1980), it is thought to be at least 2m from the source, based on what has been reported in other studies, and due to the dangers of sampling close to source in the composting environment. As already discussed, ideally concentrations should be taken directly at the source of emission, as the pollutant disperses and becomes diluted immediately upon release (Beychok, 1994).

This method of emission rate calculation is not possible within the context of this study, due to the ADMS model developers not releasing the equations and algorithms used by the model. Even if this information was known to the modeller, it would still be difficult to apply this method to the composting scenario due to the lack of knowledge surrounding many model inputs, as discussed in more detail below.

Back extrapolation

Back extrapolation, sometimes referred to as retro-fitting or back calculation, is the process of obtaining an emission rate based upon measured data. The method of back extrapolation involves adjusting the emission rate model parameter until the modelled outputs resemble some measured concentration data (Danneberg *et al.,* 1997; Environment Agency, 2001b; Taha and Pollard, 2004; ADAS, 2005; Taha *et al.,* 2006; 2007; SNIFFER, 2007; Tamer Vestlund, 2009). This approach is subject to similar limitations as the emission rate calculation method, in particular limitations 2 and 3.

Due to the limitations of back extrapolation, this method has not yet been successful in modelling bioaerosols from composting facilities. This method may be possible once some of the limitations are addressed; for example, once other model inputs have been quantified and measurements close to source have been improved.

2.5.2 Source geometry

Point (Millner *et al.,* 1980; Danneberg *et al.,* 1997; Taha and Pollard, 2004; Taha *et al.,* 2006; 2007; Drew *et al.,* 2007; SNIFFER, 2007; Tamer Vestlund, 2009), area (ADAS, 2005; Taha *et al.,* 2006; 2007; SNIFFER, 2007; Tamer

Vestlund, 2009) and volume sources (Environment Agency, 2001b; Taha *et al.,* 2006; SNIFFER, 2007) have all been modelled, to represent different compost site processes and features. The geometrical dimensions previously modelled for each source type is discussed below. It is very difficult to estimate the dimensions of bioaerosol releases at open windrow composting facilities during agitation activities as emissions are not contained or controlled. It is not possible to directly measure the area of the agitation due to the dangers associated with sampling close to source (Taha *et al.,* 2006) as previously discussed. However it is possible to estimate and justify the dimensions of the source based on personal observations, similarly to Millner *et al.* (1980) and Taha *et al.* (2006), or by using the technical specifications of the agitation machinery used.

Point source

Point sources are normally used to represent pollutant stacks (SNIFFER, 2007) where the dimensions of the stack are well defined and easy to measure. In the context of bioaerosol emissions from agitation activities at composting facilities, point sources have been used to represent agitation activities, such as screening, turning, loading, shredding and vehicular movements (Millner *et al.,* 1980; Danneberg *et al.,* 1997; Taha *et al.,* 2006; 2007; Drew *et al.,* 2007; SNIFFER; 2007). The geometry of the source modelled has not been stated in many of the studies summarised in Table 2-6 (Danneberg *et al.,* Drew *et al.,* 2007; SNIFFER 2007). Of those studies where source dimensions have been stated, the height of the emission modelled has ranged from 0 to 5 metres (Millner *et al.,*1980; Taha and Pollard; 2004; Taha *et al.,* 2006; 2007; Tamer Vestlund, 2009). Only two of these studies has justified the emission height modelled. Millner et al. (1980) based the 5 metre modelled height of emission on observations of smoke plumes generated from flares attached to the machinery, whereas Taha *et al.* (2006) modelled with a 0 metre height of emission based on observations of the agitation activity. Modelled source diameter has been stated in only two studies in Table 2-6 (Taha *et al.,* 2006;

2007). Both studies modelled with a diameter of 3 metres, although it is not justified why this assumption was made.

Area source

An area source is a release over a horizontal plane at a specified height, and the emission is assumed to be uniform across the area (CERC, 2010b). An area is often used to represent pollutant emissions from sewage tanks or landfill (CERC, 2010b), where the dimensions of the emission are known and easily measurable. As summarised in Table 2-6, area sources have been used to represent the area covered by the portable wind tunnel when measuring static emissions (Taha *et al.,* 2006; 2007; Drew *et al.,* 2007; SNIFFER 2007; Tamer Vestlund, 2009), or an agitation activity (ADAS, 2005). Focussing on modelled emissions for agitation activities from open windrow facilities, the dimensions used in the ADAS (2005) study were 10 by 2 metres with a height of 1.8 metres. ADAS (2005) admitted that these values were arbitrary, but also believed that they were a fair approximation of emissions.

Volume source

Volume sources are often used to represent fugitive emissions from buildings (CERC, 2010b). As summarised in Table 2-6, volume sources have been used to represent emissions from buildings at in-vessel facilities (SNIFFER, 2007), where emission dimensions was based on building dimensions. This approach cannot be applied to open windrow composting facilities as emissions are not confined to buildings, but are released in the open air.

2.5.3 Pollutant temperature

The pollutant temperature used when modelling bioaerosol emissions from open windrow composting facilities vary from 9.5 to 55°C (Taha and Pollard, 2004; Drew *et al.,* 2005; 2007; Taha *et al.,* 2006; 2007; Tamer Vestlund; 2009), as highlighted in Table 2-6. In the majority of these studies, the modelled pollutant temperature has not been justified. Only the studies by Drew *et al.* (2005) and Tamer Vestlund (2009) have stated where the pollutant temperature modelled has arisen. The pollutant temperature modelled by Drew *et al.* (2005)

was 17.5°C, and was the measured ambient temperature on the day of sampling. Tamer Vestlund (2009) also used measured ambient temperatures as values for pollutant temperature within the model. Although justified, this is likely to be incorrect as it is well recognised that the cores of composting windrows can reach temperatures of up to and beyond 55-60°C (Lacey and Crook, 1988). Tamer Vestlund (2009) recognised this, and also modelled a 'high temperature scenario' using a pollutant temperature of 55°C. However, as the core of the windrow is exposed during agitation activities, the temperature is expected to drop rapidly, but still remain above ambient temperature, allowing the pollutant plume to rise. This is because the hot less dense air at the core of the windrow is exposed to the cooler ambient air, causing the air, and all pollutants contained within it, to rise and rapidly decrease in temperature. This is illustrated in Figure 2-4.

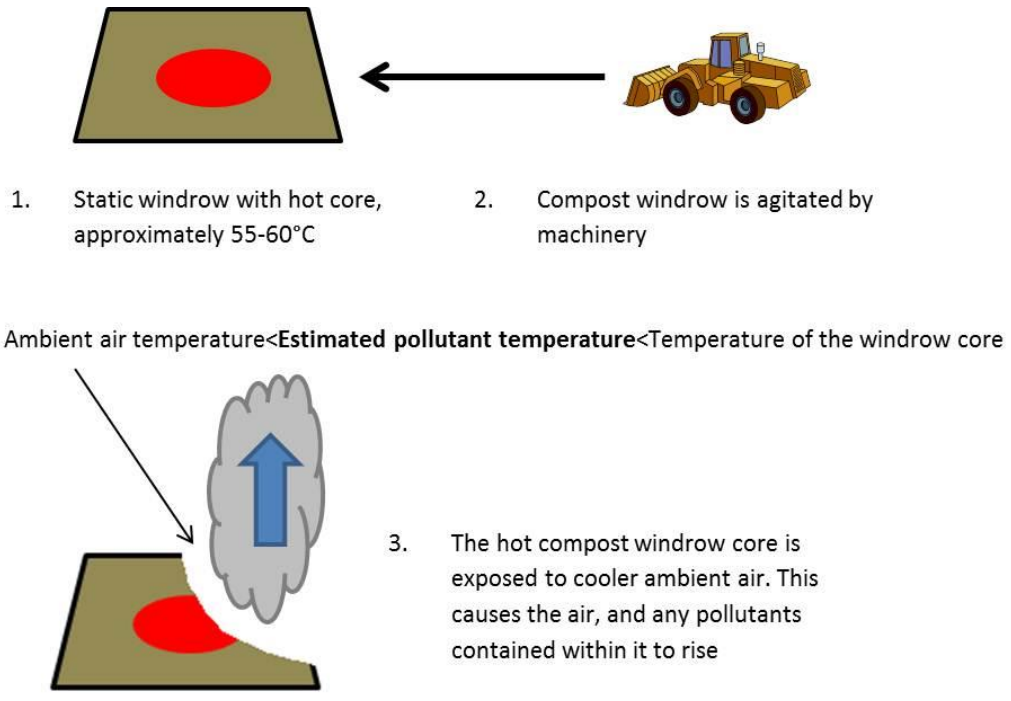

Figure 2-4 Schematic of pollutant temperature at source of bioaerosol emission

Due to the dangerous nature of the composting activities, it has not yet been possible to measure source characteristics. Therefore, at present, there are no known measurements or reliable estimations of the temperature of bioaerosol emissions from agitated compost windrows.

2.5.4 Pollutant exit velocity

Literature on the exit velocity of bioaerosol emissions from composting activities is very limited. Drew *et al.,* (2005), Taha *et al.,* (2007) and Tamer Vestlund (2009) modelled with a velocities of 0.19, 0.2, and 0.5-1.7 metres per second respectively, as highlighted in Table 2-6, but it is not apparent how these figures were estimated, calculated or measured. All other studies where active bioaerosol emissions from composting facilities have been modelled do not state what exit velocity was used, if any. Miller *et al.,* (1980) and Dowd *et al.,* (2000) estimate emission rates via equation rearrangement using the model of Pasquill, or modified versions of it. This model requires a mean ambient wind speed and not a pollutant exit velocity. Therefore, at present there are no known measurements or reliable estimations of bioaerosol exit velocity from agitated compost windrows.

2.5.5 Meteorological inputs

As portable weather stations are readily available, and can be used safely on site, theoretically all modelling studies should contain accurate meteorological data. However, only a handful of studies have reported what meteorological conditions were modelled, if any at all, as highlighted in Table 2-6. The AfOR protocol (2009) states that meteorological conditions should be monitored, thus meteorological conditions should be available when modelling more recent bioaerosol datasets. Accurate meteorological inputs are paramount when modelling scenarios, as they determine pollutant dispersal and transport (Oke, 1987).

Ambient wind speed determines the rate at which the pollutant is dispersed, and also has effects on plume rise and turbulent activity (Oke, 1987). Higher wind speed result in more turbulence, more rapid dispersal and less plume rise (Oke, 1987). Ambient wind speeds are the most commonly reported model inputs in the studies, ranging from 0.1 to 8.9 metres per second (Millner *et al*., 1980; Dowd *et al.,* 2000; Taha and Pollard *et al.,* 2004; ADAS, 2005; Taha *et al.,* 2006; SNIFFER, 2007) as reported in Table 2-6. Although this is not a huge range, Oke (1987) points out that an increase in wind speed from 2 to 6 metres

per second can lead to much quicker dispersal and therefore lower pollutant concentrations downwind. This is because the volume of air passing the source of emission per unit time is larger. Modelled ambient temperatures are not reported in many studies. Only Taha *et al.,* (2006) and Drew *et al.,* (2005) have reported modelled ambient temperatures of 16.3-19.3ºC and 17.5°C respectively. Ambient temperatures affect the amount of plume rise and therefore dispersion, as already discussed in section 2.5.3. ADAS (2005) and Tamer Vestlund (2009) are the only studies in Table 2-6 to report a surface roughness, which was 0.2 metres relating to agricultural land. Surface roughness affects boundary layer turbulence, and therefore pollutant dispersal. ADMS gives several surface roughness options, based on land-use (CERC, 2010b), and thus can be easily estimated.

Although the meteorological conditions used when modelling the dispersion of bioaerosols have been reported more frequently than other model input parameters, it is still unclear how these values were measured or estimated.

2.5.6 Sensitivity analysis

As highlighted above, there are many gaps in knowledge surrounding many different model inputs. It is important that the model inputs are accurate and well justified for the scenario being modelled; otherwise model outputs may be incorrect. Due to the difficulties and expense of measuring these parameters, a sensitivity analysis [SA] could be carried out to prioritise which parameters need to be quantified. A SA is the study of how variation in the outputs of a computational model can be apportioned qualitatively or quantitatively to variation in the model input parameters (Saltelli *et al.,* 2000; Ligmann-Zielinska and Jankowski, 2008; Li *et al.,* 2010). Many SAs have been performed on various dispersion models previously (Mensink and Maes, 1997; Futter, 2000; Xing *et al.,* 2007; Giambini *et al.,* 2008; Harsham and Bennett, 2008; Tamer Vestlund, 2009; Zou, 2010; Pandya *et al.,* 2012). However, these SAs have often been performed on parameters and ranges not applicable to the open windrow composting scenario, as described in more detail in section 3.3. Therefore a SA specific to the open windrow composting scenario should be

completed. This would identify what the key inputs are within the dispersion model, within this specific scenario, providing an order of prioritisation when improving input parameter quantification.

2.6 Key gaps in knowledge and objectives

2.6.1 Scenario specific sensitivity analysis

Many model inputs are approximated due to the lack of input information as highlighted in section 2.5.6. However it may not be possible to collect all of the data needed to use as inputs in the model due to:

- Risks associated with sampling on-site, especially close to sources of compost agitation
- Methods needed to collect the data may not exist
- Cost and time constraints

However it may not be necessary to quantify all of the unknown parameters in the model, as some parameters may have little effect of the model outputs. Therefore a sensitivity analysis specific to the open windrow composting scenario can be performed to identify which input parameters affect the model outputs the most. This would give an order of prioritisation when quantifying the unknown inputs. Sensitivity analyses have been performed on dispersion models prior to this study (Mensink and Maes, 1997; Futter, 2000; Xing *et al.,* 2007; Giambini *et al.,* 2008; Harsham and Bennett, 2008; Tamer Vestlund, 2009; Zou, 2010; Pandya *et al.,* 2012). however these have been performed on input parameters and ranges irrelevant to this specific scenario and thus is needs to be repeated, in the context of the open windrow composting scenario.

Objective 1

To perform a sensitivity analysis, specific to the scenario of bioaerosol emissions from open windrow composting facilities, to determine which input parameters affect the model output concentrations the most.

This objective will be addressed in Chapters 3 and 4. The purpose of Chapter 3 will be to reduce the amount of inputs and input ranges within the SA by

completing a screening stage, which will also reduce the amount of data analysis in the SA. Chapter 4 will use the information from Chapter 3 to complete the SA in full.

2.6.2 Scenario specific model calibration and validation

Although the ADMS dispersion model has been well tested and validated, (Carruthers *et al.,* 1993; 1994b; 1995; 1998; 2001; 2005; Hanna *et al.,* 2000; CERC 2010) an open windrow composting scenario specific model calibration and validation has never been completed. A model calibration and validation tests the reliability of the model outputs when compared to a set of measured data (Sahraoui and Jayakrishnan, 2005). Model calibration and validation has not been possible on the ADMS model in the composting scenario due to a lack of measured data, as described in section 2.3.4. However, an extensive set of measured data is now available, collected by Pankhurst (2010), and this model calibration and validation is now possible.

Objective 2

To complete a model calibration and validation, in the context of bioaerosol emissions from open windrow composting facilities, using existing sets of measured data.

This objective is addressed in Chapters 5,6 and 7. Chapter 5 describes the model calibration, and Chapters 6 and 7 describe the model validation.

2.6.3 Dispersion model input improvements

Dispersion models have not yet been successful at accurately estimating bioaerosol concentrations emitted from open windrow composting facilities. This has been caused by:

- A lack of a comprehensive dataset of bioaerosol concentrations measured downwind of a composting facility, to use when testing the performance of the dispersion model in the open windrow composting context.

- Limited data on potentially key aspects of the emission properties, thus giving a lack of confidence of what values to use for certain inputs to the dispersion model

Dispersion model inputs including emission rate, pollutant temperature, and pollutant exit velocity have not been well defined or justified in current modelling studies, particularly when modelling agitation activities where higher bioaerosol concentrations are expected (Taha *et al.,* 2006). If the dispersion model is run with unreliable model inputs, then the model outputs will be unreliable also. Collection of data at open windrow composting facilities is challenging as emissions are uncontrollable and are not contained. It is also difficult and dangerous to collect data during agitation events, due to the machinery used to complete these activities. This had led to many model input estimations, or model inputs based on samples collected away from agitation activities.

Objective 3

To collect data, using novel techniques and existing data collection methods if possible, to improve the knowledge of selected dispersion model inputs, in the open windrow composting context, to provide more accurate modelled output concentrations.

This objective is addressed in Chapter 8. It should be noted that information from the completion of Objective 1 in Chapters 3 and 4 was used to decide what inputs to quantify in Chapter 8. Equally, the emerging results from completing Objective 3 in Chapter 8 were used to justify decisions made in Chapters 3, 4, 5,6 and 7. This is illustrated in Figure 1-1.

2.6.4 Best-practise modelling recommendations

Using the information provided by completing objectives 1, 2 and 3, a best practise modelling protocol can be produced when modelling bioaerosol emissions from open windrow composting facilities. This can aid other model users to accurately simulate bioaerosol emissions in this unique context. If bioaerosol emissions from open windrow composting facilities can be simulated with confidence, then the model could be used in several other applications. For

example, it could be used as a useful tool in the waste permitting process, to provide continuous bioaerosol concentration data when assessing the risk of bioaerosol exposure to nearby sensitive receptors.

Objective 4

To create best-practise modelling recommendations when using dispersion models to accurately estimate bioaerosol emissions from open windrow composting facilities.

This objective is addressed in Chapter 9.

3 Sensitivity analysis screening stages

3.1 Introduction

The previous chapter identified the key gaps in knowledge surrounding the modelling of bioaerosol emissions from green waste composting facilities. One of the key gaps in knowledge was associated with the lack of justified model inputs. This has occurred due to a lack of measurement and knowledge surrounding bioaerosol emissions from open windrow composting facilities. Therefore more research is required to provide credible inputs within the dispersion model.

There are two main types of SA, namely local and global (Saltelli *et al.,* 2000). Briefly, a local SA examines the variability of the model outputs when varying the model input parameters one at a time, holding all other parameters at a constant value. This is also known as the one at a time [OAT] method (Xu and Gertner, 2007). A global SA focuses on the output variability over the specified range of values of the input parameters, when altered altogether (Homma and Saltelli, 1996). SAs are useful because:

- They increase the understanding of the model by giving insight into the relationships between input and output variables (Pannell, 1997; Ireland *et al.,* 2004)
- They identify critical values and sensitive/important variables (Pannell, 1997; Ireland *et al.,* 2004), and determine which parameters need further quantification for model validation (Hamby, 1994)
- They can help during development stages of the model, particularly during model calibration and validation. Furthermore it can provide insightful information where data is partial or missing (Pannell, 1997; Ireland *et al.,* 2004)

Therefore a SA will be particularly useful in the open windrow composting scenario. A SA can be used as a tool for determining the most sensitive model input parameters for this unique scenario, providing information on what model parameters require further research or quantification most urgently. This is

particularly useful as bioaerosol data collection can be very costly and time-consuming. SAs can also aid with the model calibration process, providing a structured order in which model adjustments are completed.

The dispersion model, ADMS, will be used throughout the project, and is justified and described in sections 3.2 and 3.2.1. ADMS has a large number of input parameters, which can be inputted within the model interface or included as separate files. Incorporating separate files in a SA of the ADMS model is technically difficult, and thus a screening stage was completed prior to the main SA. A screening stage determines which input variables are significantly contributing to output concentration, but does not quantify which parameters are more sensitive than others (Morris, 1991; Campolongo *et al.,* 2007). A screening stage can be used to decrease computational running times and reduce the number of input parameters included in a SA. Consequently this reduces the amount of data analysis. The model inputs and parameter ranges included in the screening stages are representative of conditions observed at open windrow composting facilities.

3.2 Dispersion model justification

In this project a Gaussian dispersion model will be used, as justified in section 0. The dispersion model used in this study must be appropriate for modelling bioaerosol emissions from open windrow composting facilities. Some facilities are situated on complex terrain, such as in or near to valleys, or steep land, and thus models that are not capable of modelling the effects of terrain are not suitable. Additionally, as composting facilities are sometimes located near to buildings, particularly in urban environments, the dispersion model chosen must also be capable of modelling the effects of buildings. This eliminates the use of the ISC/ISCST3, SCREEN and AUSPLUME models from this study (Simms *et al.,* 2000; Ministry for the environment, 2004; US EPA 1995b), as highlighted in Table 2-5. Due to current bioaerosol threshold values recommended by the Environment Agency (Environment Agency, 2001b), there is particular interest in bioaerosol emissions, dispersal and concentrations within the first 250 metres of the composting facility. Therefore the model chosen must be capable of

accurately predicting emissions within close vicinities of the emission source. This thus eliminates the use of the CALPUFF model in this study as it has been reported that it may provide a less accurate estimation of pollutant emissions within close proximities of the source (Hoffnagle, 2008; Dionne, 2011).

Therefore the choice of dispersion model must be between AERMOD and ADMS. ADMS is the preferred choice of model when modelling pollutant emissions in the UK (Hall *et al.,* 2000b), whereas AERMOD is a preferred choice in the USA (US EPA, 2012c). In inter-model comparison studies, ADMS and AERMOD have performed similarly when comparing modelled outputs to measured data (Hanna *et al.,* 2000; Hall *et al.,* 2000a; 2000b). This is probably due to the similarities in the way the atmospheric boundary layer is described by using the Monin-Obukhov length (Carruthers *et al.,* 1994; McHugh *et al.,* 1999; Riddle *et al.,* 2004), and the fact that the models use many of the same algorithms (Hanna *et al.,* 2000). Hanna *et al.,* (2000a) directly compared the outputs of ADMS and AERMOD to the measurements taken at five different field sites. It was concluded that ADMS performed slightly better than AERMOD (Hanna *et al.,* 2000a). Based on this information and the fact this study will utilise bioaerosol measurements sampled from facilities in the UK, the dispersion model ADMS (version 4.2) will be used throughout this study.

3.2.1 ADMS model description

ADMS has been well tested and validated (Carruthers *et al.,* 1993; 1994b;1995; 1998; 2001; 2005; Hanna *et al.,* 2000a; CERC 2010) and a full description of the model can be accessed via the model developers website (CERC, 2012). However the model has never been calibrated and validated in the context of bioaerosol emission from composting facilities. ADMS is a ‘black box’, in other words, the equations and algorithms that the model uses to convert the model inputs into output concentrations are not shown. However it should be noted that some equations used within the model are described in the technical specifications for different aspects of the model (CERC, 2012).

ADMS, like all dispersion models, requires some basic inputs. The minimum requirements of the model depend on what meteorological information is

available, and what efflux type is modelled (CERC, 2010b). Based on an exit velocity efflux, the main inputs required to run the model are:

- Source type and corresponding dimensions, including source height
- Pollutant emission rate, exit velocity and temperature
- Latitude and surface roughness of the dispersion or meteorological measurement site
- Wind speed and angle and
    - Surface heat flux or
    - Cloud cover, year, day and time
- Averaging time (CERC, 2010b)

The model allows the user to employ the default values available in the model. However, all inputs used should be representative of the scenario modelled, to allow more accurate estimations of reality.

Figure 3-1 provides a screenshot of the ADMS model interface, which illustrates the simplicity of the software, and highlights the key input tabs in the model.

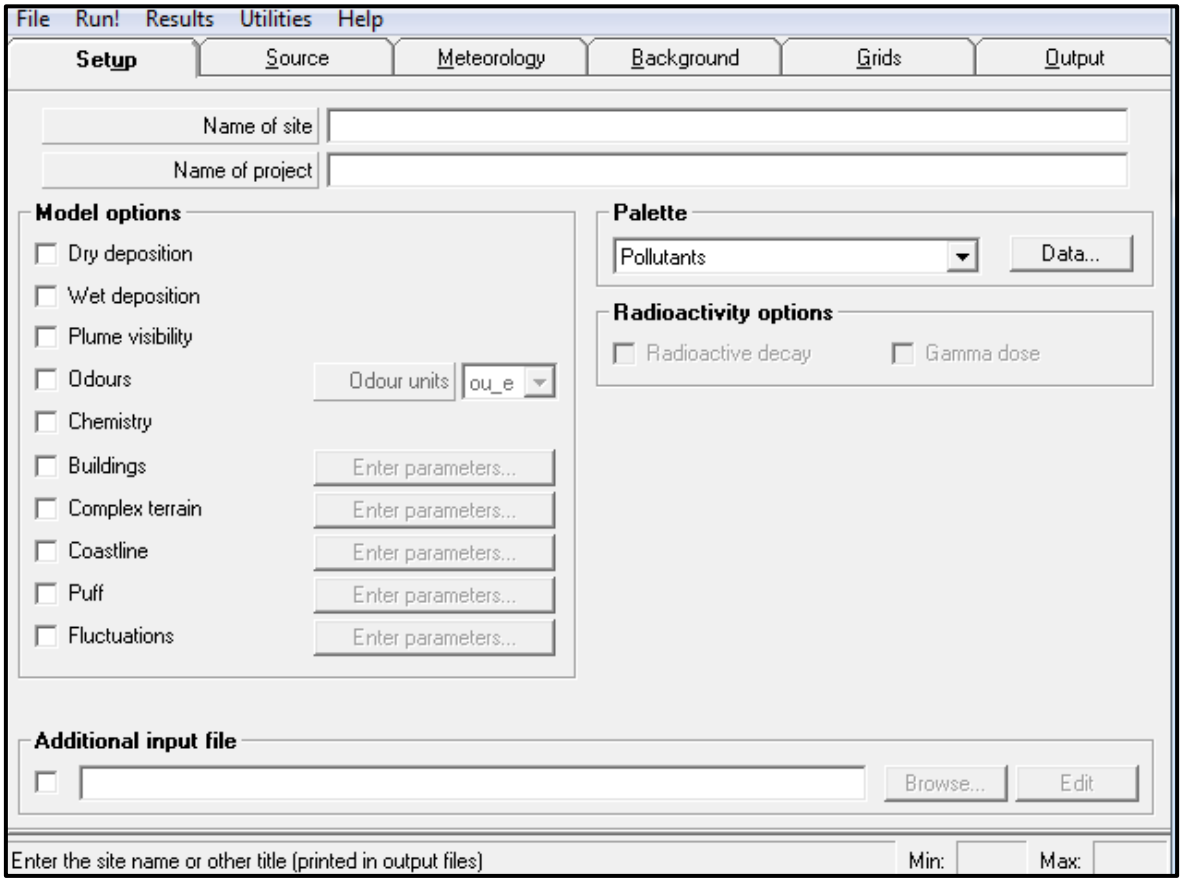

Figure 3-1 A screenshot of the ADMS model interface. The key input tabs 'Setup', 'Source', 'Meteorology', 'Background', 'Grids' and 'Output' can be seen at the top of the screenshot.

3.3 Previous sensitivity analysis studies performed on ADMS

Multiple general SAs have been performed on different aspects of ADMS prior to this study (Mensink and Maes, 1997; Futter, 2000; Harsham and Bennett, 2008; Tamer Vestlund, 2009). These are summarised below:

- Mensink and Maes (1997)

  A sensitivity study on ADMS was performed, considering SO_2 emissions only, from a hypothetical coal-fired power plant, with a stack height of 110 metres. Input parameters such as stack height, emission rate, and pollutant temperature were altered within fixed ranges one-at-a-time

[OAT]. Sensitivity indicators were defined, relating to the standard deviation of the parameter variations, to determine the sensitivity of each input parameter. Emission rate, pollutant temperature and source height were all sensitive parameters.

- Futter (2000)

  Only meteorological inputs were included in the SA performed by Futter, in the context of SO_2 emissions from high stack power stations. Futter altered wind speed, cloud cover, heat flux and the boundary layer height within defined ranges. Futter (2000) does not clearly state whether this analysis was performed OAT or not. Futter (2000) found that all of these parameters were sensitive.

- Harsham and Bennett (2008)

  A SA was conducted in the context of an industrial plant with a 30 metre stack height. The study suggests that the surface roughness was altered between 0.03 and 1.00, although this is not clear. It is also unclear whether the SA was performed using a OAT method, and what parameters, if any were sensitive.

- Tamer Vestlund (2009)

  Tamer Vestlund (2009) varied many model inputs parameters OAT, including parameters associated with the source and meteorological inputs. This SA was intended to be specific to the bioaerosols from open windrow composting context. However, parameters were altered in multiples of 10, 100 or 1000 from base values where possible, thus including input values not applicable to this context. The majority of the source and meteorological parameters were sensitive, although pollutant properties were not. After evaluating this study, it is apparent this has been a caused by modeller error, as the wet and dry deposition parameters were not used, and thus changes in the pollutant properties were not considered.

However, these SAs were mostly performed on parameters and within inputs ranges that were often not applicable to the open windrow composting scenario. For example, Mensink and Maes (1997) tested stack heights of 50 to170

metres, which are impossible in the open windrow composting context. Additionally, in some of the studies, a large range of possible inputs for a particular input parameter were included, but few values were tested, resulting in a SA with low resolution. For example, Tamer Vestlund (2009) altered parameters in factors of 10, 100 and 1000 where possible from a fixed central value. This resulted in three very different source heights of 3, 30 and 300m being tested in the SA.

The SA screening stages and main SA presented in this chapter, and the following chapter respectively, describe a scenario specific SA performed on input parameters and input parameter ranges relevant to the bioaerosol emissions from open windrow composting facilities situation. This will improve on previous SAs by:

- Including input parameters and input parameter ranges relevant to this specific scenario only
- Including more values in the specified input parameter ranges to improve resolution
- Changing all of the input parameters, either OAT or together, relevant to the open windrow composting scenario, instead of changing a few selected parameters

This will improve the understanding of which input affect the modelled outputs the most, in the open windrow composting scenario. This information can be used to provide precedence to:

- Which model inputs are adjusted primarily in the model calibration (chapter 5)
- The improved quantification of selected model input parameters (chapter 7)

3.4 Methods

The screening stage was divided into two parts, including a meteorological stage and an uncertainty stage. In both cases, the inputs and ranges used were

based on realistic possibilities in the scenario of bioaerosol releases from composting facilities.

Screening stage one was performed on the meteorological parameters. There are many meteorological options available within the dispersion model, and can be inputted within the model interface or as a separate file (CERC, 2010b). Only selected meteorological inputs and up to 99 lines of meteorological data can be entered within the model interface (CERC, 2010b), and therefore it was opted to input the parameters via a separate meteorological file. As entering the meteorological data via a separate file would result in a more technically complex sensitivity analysis, resulting in long computational times, an analysis of the sensitivity of the meteorological data is assessed in this chapter, separately to the main SA.

As there is limited knowledge surrounding bioaerosol emissions from open windrow composting facilities, there are many uncertainties surrounding what input values should be used for certain model input parameters when modelling this scenario. In other words, the input values for some model parameters cannot be justified within the open windrow composting context. As a consequence of this uncertainty, it would be necessary to include the whole possible range that the dispersion model allows within the SA. On the other hand, there are some parameters in which the whole range allowed in the dispersion model is applicable to the open windrow composting scenario. It is undesirable to include the whole input ranges, as the resolution of the main SA would be reduced. Therefore screening stage two was performed to determine which of these parameters and parameter ranges are sensitive. This can potentially reduce the number of model inputs and ranges included in, and increase the resolution of, the main SA.

At this stage, only steady-state, non-episodic emissions are modelled for two reasons:

- To keep the model running times and time required to analyse the data to a minimum

- At present there is not enough data or information to input the information required to model episodic emissions with accuracy

Therefore the source of the emission is represented as a singular point source, based on the inputs used in the dispersion modelling completed by Millner *et al.,* (1980); Danneberg *et al.,* (1997); Dowd *et al.,* (2000); Environment Agency, (2001b); Taha and Pollard (2004); Drew *et al.,*(2005; 2007); Taha *et al.,* (2006; 2007); SNIFFER, (2007); Tamer Vestlund (2009).

3.4.1 Screening stage 1 – meteorological inputs

Screening stage 1 was performed on meteorological variables relevant to this scenario and expands on the simple OAT method used by Tamer Vestlund (2009). The meteorological parameters were entered into ADMS via a separate file. Remaining parameters located within the main model interface were held at constant values, based on values previously used within dispersion models when modelling the dispersion of bioaerosols from composting facilities, as detailed in Appendix 1.

Modelled concentration outputs were given at 10, 100 and 250 metres downwind of the modelled source at a height of 1.7 metres (corresponding to breathing height) on the plume centreline. Each parameter included in the analysis was assigned a minimum and maximum value, based on historical weather conditions measured throughout the UK (Oke, 1987; Willet *et al.,* 2008; Met Office, 2011a). Additionally a baseline value was assigned for each parameter, reflecting the most likely occurrence in the UK, also based on historical UK weather conditions (Willet *et al.,* 2008; DECC, 2011; Met Office, 2011a). Parameters were altered incrementally around the baseline value. The parameters, ranges, baseline values, and incremental changes included in the screening stage are shown in Table 3-1. Although the ranges and baseline values are based on observed meteorological conditions, the values used in the meteorological file are artificial. Excluded parameters are variables that are not normally entered by the model user, where a default value is used or the value is estimated by the model based on other inputs (CERC, 2012). Parameters were changed OAT whilst keeping all other parameters held fixed at their

baseline values. To detect any possible interactions between meteorological inputs, two or more parameters were also altered in unison whilst the remaining parameters were held at their baseline values. This resulted in a meteorological file consisting of the equivalent of over 24 years of meteorological data (over 9000 days). The actual values used in the meteorological file are provided in the data disc. A summary of the method used to complete screening stage 1 is illustrated in Figure 3-2.

Table 3-1 Meteorological parameters, ranges and baseline values included in screening stage one

Parameter (Units)	Range	Range Justifications	Baseline value	Baseline value justification	Incremental change
Wind speed (m/s)	0-36.5	The upper value was based on the highest hourly mean wind speed recorded in the UK (Met Office, 2011b). The lower value represents zero wind.	3	Based on an estimation of ground –level annual mean wind speeds in the UK (DECC, 2011)	0.25
Sensible heat flux (W/m^2)	-50-120	Sensible heat flux is not routinely measured at weather stations throughout the UK (Met Office, 2013). Therefore this range was based on existing optional meteorological files included within ADMS	0	Based on the sensible heat flux observed during the neutral atmospheric stability class (Middleton, 1996)	1
Boundary layer depth (m)	90-2000	According to Oke (1987), the boundary layer depth can extend to 2000m by day and shrink to less than 100m by night	1000	Boundary layer depths are not routinely measured in the UK (Met Office, 2013).Therefore a mid-range value was used	10
Cloud amount (oktas)	0-8	Maximum range allowed within the dispersion model	4	Cloud levels constantly change in the UK, therefore the median of the range was used as a baseline value	1

Parameter (Units)	Range	Range Justifications	Baseline value	Baseline value justification	Incremental change
Ambient temperature (°C)	-27-38.5	Based on the lowest and highest recorded ambient temperatures recorded in the UK (Met Office, 2011c; 2011d)	9	Based on the annual mean temperature in the UK between 1981-2010 (Met Office, 2011e)	0.1
Relative humidity (%)	50-90	According to Willet *et al.* (2008), relative humidity tends to be higher in higher latitudes, like the UK	80	Based on the climatological mean for the UK between 1974-2003 (Willet *et al.,* 2008)	1

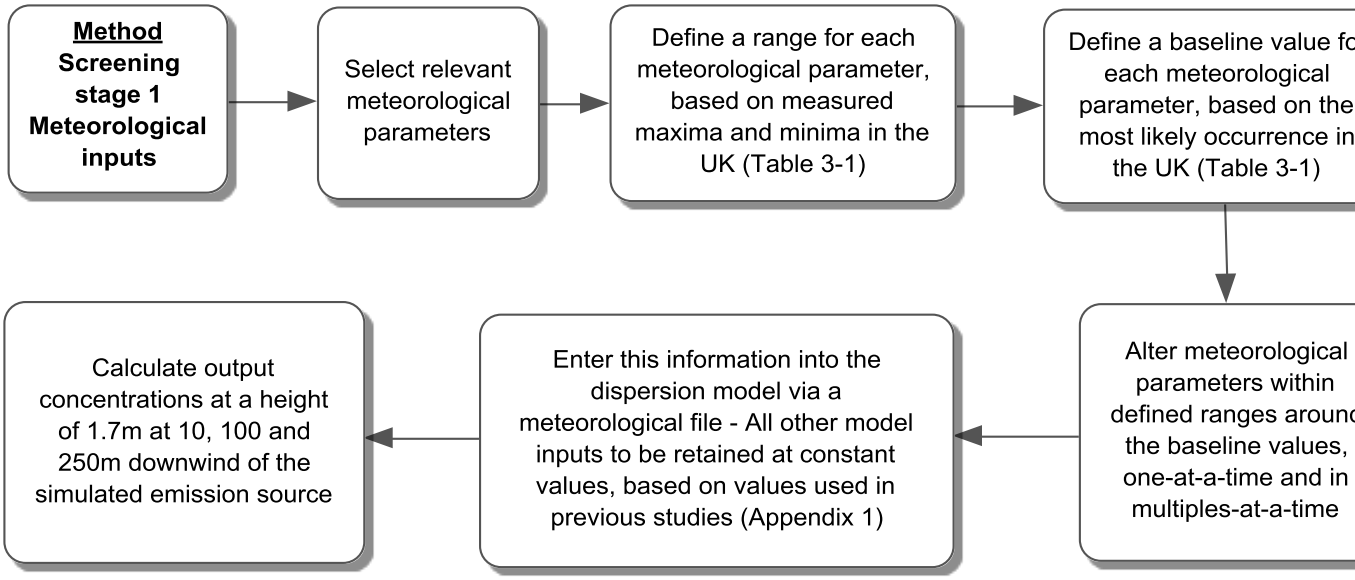

Figure 3-2 A summary of the methods used to complete screening stage 1

The purpose of the screening stage was to reduce the amount of meteorological data included in the main SA. To do this, key meteorological inputs were determined by observing graph gradients. The gradient of the graph indicates the rate at which the model output concentrations change with respect to the input parameters, or in other words, the sensitivity of a parameter. Key model input values could be identified at points on the graph where the gradient had changed significantly. The model input values where the gradient changed significantly could then be identified. These values were then used to create the meteorological file for use within the main SA run. This is illustrated in

Figure 3-3.

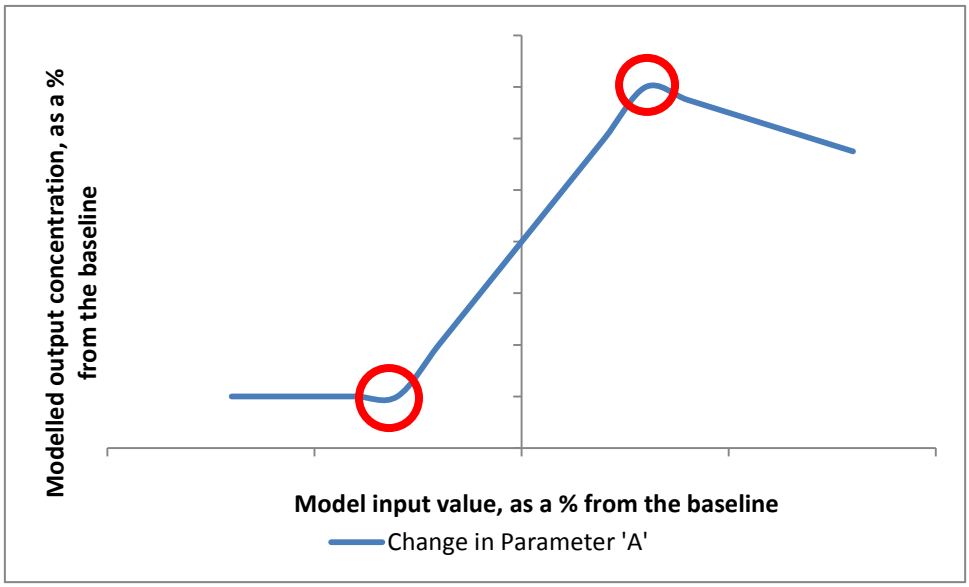

Figure 3-3 Example of how gradient analysis can identify key model inputs. The red circles identify where the gradient of the graph has changed significantly, thus indicating sensitive input ranges for a particular parameter.

3.4.2 Screening stage 2 – analysis on selected input parameters

Screening stage 2 is a development of, and utilises the results achieved from screening stage 1. Screening stage 2 was performed on input parameters in which there is limited knowledge or data, or on input parameters in which the maximum allowed range within the dispersion model was relevant to the open windrow composting scenario. The lack of data or knowledge surrounding these parameters became apparent when justifying the parameters and ranges to be included within the main SA. Similarly, the ranges in which the maximum range allowed within the model was found to be applicable to the open windrow composting scenario, was determined when justifying the inputs and ranges included in the main SA. This screening test was devised to reduce the range, or eliminate the inclusion of the selected parameters, relevant to the open windrow composting context, from the main SA, to increase the resolution of the main SA.

Again, an OAT method was used, but random numbers were generated for each parameter range instead of input parameters being altered incrementally.

The Microsoft® Excel add-in @Risk© (Palisade, 2011) was used to generate the random numbers within a probability distribution. As the values for the input parameters are uncertain, a uniform distribution was assigned to each input parameter, whereby every value across the specified range has an equal likelihood of occurrence (Palisade, 2009). The meteorological inputs created from screening stage 1, as described in Table 3-3 were used. All remaining parameters were held at constant values, again based on values previously used within dispersion models when modelling the composting scenario, as detailed in Appendix 1. Output concentrations were calculated at 10, 100, 250, 500, 1000, 5000 and 10000 metres downwind of the modelled source at 1.7m, corresponding to breathing height (AfOR, 2009). Parameters and ranges included in this screening analysis are described in Table 3-2, and are provided in the data disc. Table 3-2 also justifies why the parameter is included in the screening analysis.. A summary of the method used to complete screening stage 2 is illustrated in Figure 3-4.

The data was analysed similarly to screening stage 1 (section 3.4.1). A low or flat gradient indicates that a parameter is not sensitive. Following this principle, the gradient can be used to indicate when a particular parameter input, or input range is sensitive.

.

Table 3-2 Model parameters and ranges included in screening stage 2, with justification

Parameter (Units)	Justification of inclusion	Range used	Justification of range
Pollutant exit velocity (m/s)	Section 2.5.4 in Chapter 2, highlighted the fact that the pollutant exit velocity has not been measured within the open windrow composting context. Therefore there is no current evidence to suggest what the pollutant exit velocity of bioaerosol emissions from open windrow composting facilities is.	0-100	The possible range allowed in the model is 0-1000 (CERC, 2010b). To avoid low parameter resolutions, the range was reduced to 100, as it was assumed that the velocity of bioaerosol emissions will not exceed this value, based on initial observations
Pollutant specific Heat Capacity (J/°C/kg)	After an extensive literature review search, it was not possible to find any specific heat capacities for bioaerosol components. Therefore there is no current evidence to suggest what the specific heat capacity of bioaerosols or bioaerosol components is.	800-2100	The possible range allowed in the model is 0-100000 J/°C/kg (CERC, 2010b), which is a large range. To increase the resolution of the SA, the range was decreased to 800-2100 J/°C/kg, based on the specific heat capacities of common atmospheric gases (Green and Perry, 2008)
Pollutant molecular mass (g)	The molecular mass in ADMS refers to the “mass of one mole of the material” (CERC, 2010b). Overall, it is unclear what the “mass of one mole” of a bioaerosol component is.	15-45	The possible range allowed in the model is 1-300 (CERC, 2010b), which is a large range. To increase the resolution of the SA, the range was decreased to 15-45 based on the molecular masses of common atmospheric gases (Green and Perry, 2008). This range also includes the molecular mass of water, as biological cells are assumed to contain mainly water (Cooper, 2000)

Parameter (Units)	Justification of inclusion	Range used	Justification of range
Priestley-Taylor Parameter	The Priestley-Taylor parameter represents the amount of surface moisture available for evaporation, from dry bare Earth (=0) to moist grassland (=1) and beyond (CERC, 2010b). Open windrow composting facilities are located in areas of many different land types, and thus the whole range is relevant to the open windrow composting scenario	0-3	Maximum range possible within the model (CERC, 2010b), to include all surface moisture states
Minimum Monin-Obukhov length (m)	The minimum Monin-Obukhov length allows for the effect of heat production in cities (CERC, 2010b). The whole range is applicable to the open windrow composting scenario, as facilities are located in both rural and urban areas	1-200	Maximum range possible within the model (CERC, 2010b)
Surface Albedo	The surface albedo refers to the ratio of reflected solar radiation at the surface of the Earth (CERC, 2010b). Open windrow composting facilities can be located on all surface types, and thus the whole possible range is applicable to this scenario	0-1	Maximum range possible within the model (CERC, 2010b), to include all surface types

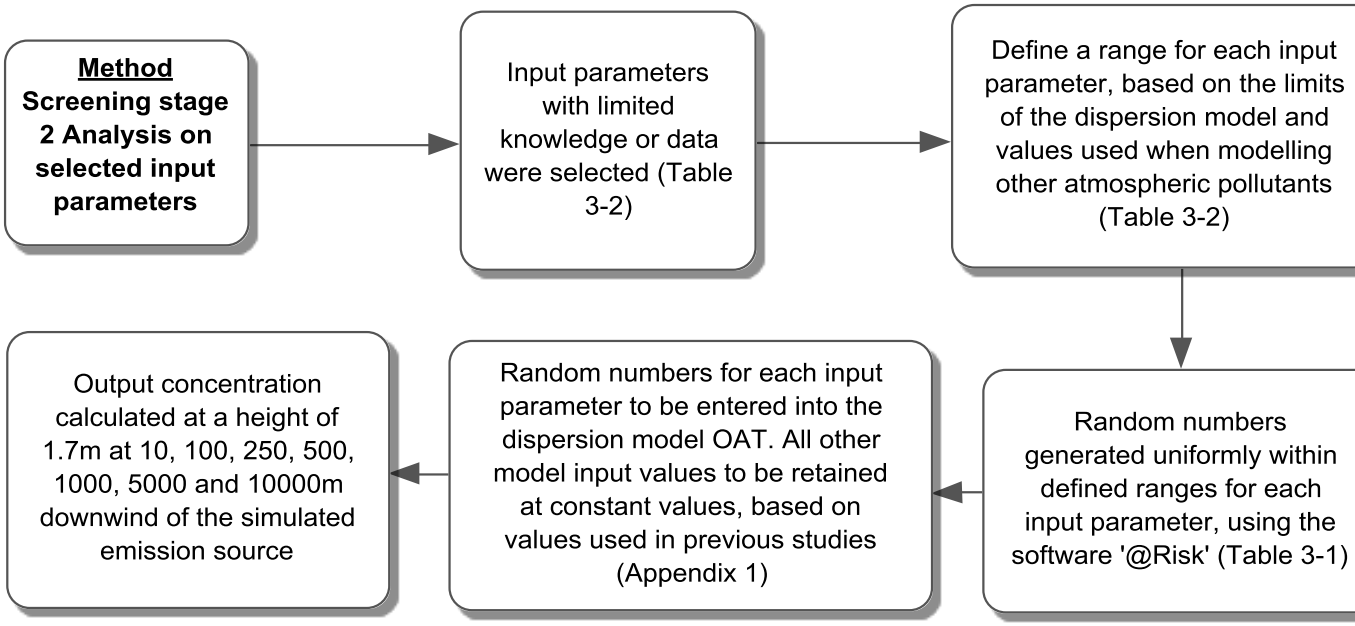

Figure 3-4 A summary of the method used to complete screening stage 2

3.5 Results

3.5.1 Screening stage 1 results – meteorological inputs

The results from OAT alterations made to the meteorological parameters, at 10, 100 and 250 metres downwind of the simulated source are presented in Figure 3-5.

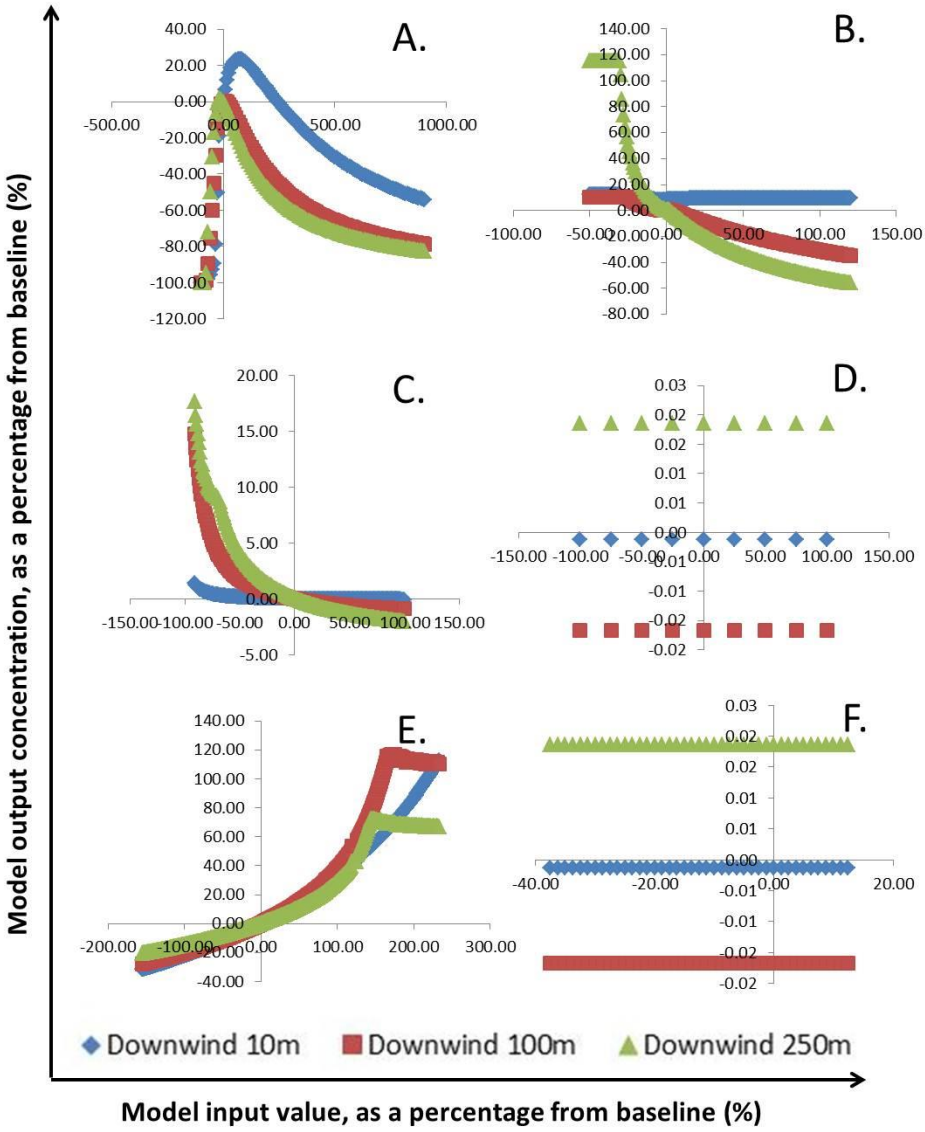

Figure 3-5 OAT changes for meteorological parameters A. Wind speed, B. Sensible heat flux, C. Boundary layer depth, D. Cloud amount, E. Temperature, and F. Relative humidity at 10, 100 and 250 metres downwind. Please note the differences in the individual graph axis scales.

As described in section 3.4.1, two or more parameters were altered in unison, and modelled outputs were calculated at 10, 100 and 250 metres downwind. This resulted in more than 150 sets of different modelled outputs, and thus these results are not presented. However, when observing the gradients of the graphs for every parameter combination at every distance downwind, general

trends emerged. The general trends are shown in Figure 3-6. Please note, that some of these general trends in the OAT changes, presented in Figure 3-5, are obscured due to the scales of the graphs. Significant Gradient Changes, [SGCs] indicating parameter sensitivity, are highlighted Figure 3-6. The model inputs at the points highlighted were identified, and were used to build meteorological scenarios.

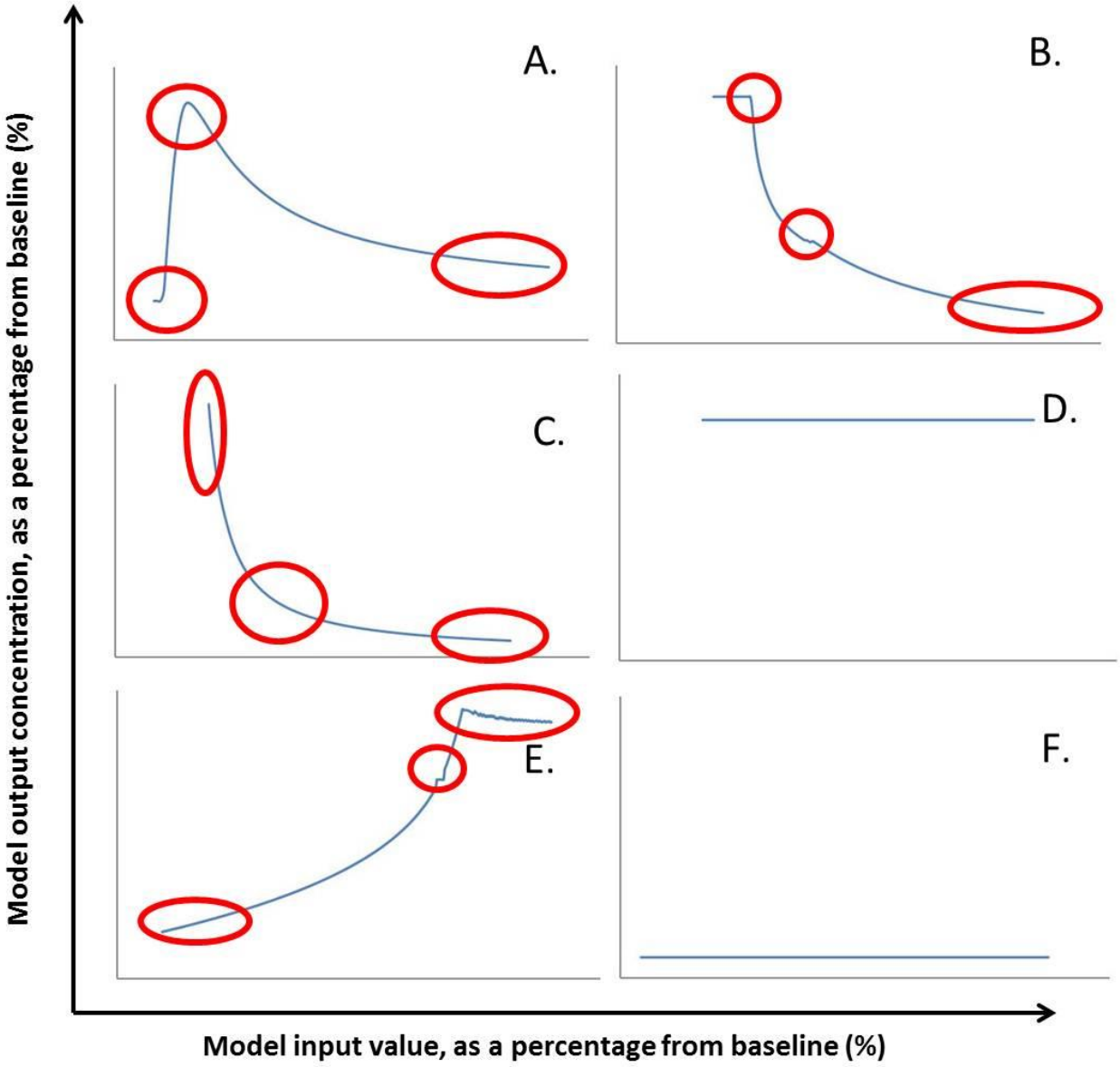

Figure 3-6 General gradient trends for A. Wind speed, B. Sensible heat flux, C. Boundary layer depth, D. Cloud amount, E. Temperature, and F. Relative humidity. Significant Gradient Changes [SGCs] are highlighted.

The inputs for the SGCs for all graphs in Figure 3-6 were observed. The gradients for graph D, cloud amount and F, relative humidity, are flat, indicating that these parameters are not sensitive. However ADMS requires thatcloud amount is included in themeteorological file to allow the model to run, and thus was included in the final meteorological scenarios. The first SGC in graphs A and E and the third SGC in graphs B and C in Figure 3-6 resulted in the lowest

output concentration, thus was named the ‘lowest concentration scenario’. The first SGC in graphs B and C, the second SGC in graph A and the third SGC in graph E in Figure 3-6 resulted in the highest output concentrations, and thus was named the ‘highest concentration scenario’. The inputs causing the second SGC in graphs B, C and E in Figure 3-6 were found to be the baseline values as reported in Table 3-1 thus creating the ‘baseline scenario’. Finally, a wind speed of 18m/s was observed for the third SGC in graph A in Figure 3-6. This was named the ‘high wind speed scenario’.. Therefore, through the completion of screening stage 1, the meteorological file has been reduced from the equivalent of over 9000 days of meteorological data, to just 4 days of meteorological data, which are now referred to as ‘meteorological scenarios’. These meteorological scenarios and input values are displayed in Table 3-3. It should be noted that parameter D,the cloud amount is included, as it is a requirement in the meteorological file (CERC, 2010b).

Table 3-3 Four meteorological scenarios, with input values, created from screening stage 1

Meteorological scenario name	Inputs				
	A. Wind speed (m/s)	B. Sensible heat flux (W/m^2)	C.Boundary layer depth (m)	D. Cloud amount (oktas)	E. Temperature (°C)
1. Lowest concentration	1	120	1400	4	-5
2. Highest concentration	5.25	0	90	4	30
3. Baseline	3	0	1000	4	9
4. High wind speed	18	0	1000	4	9

The meteorological scenarios presented in Table 3-3 will be used within the main SA run described in Chapter 4. To clarify, these meteorological scenarios are the equivalent of four lines, or four days of meteorological data.

3.5.2 Screening stage 2 results - analysis on selected input parameters

The results from the alterations made to the selected input parameters, for all meteorological scenarios presented in Table 3-3, at a distance of 10 metres downwind of the simulated source are presented in Figure 3-7.

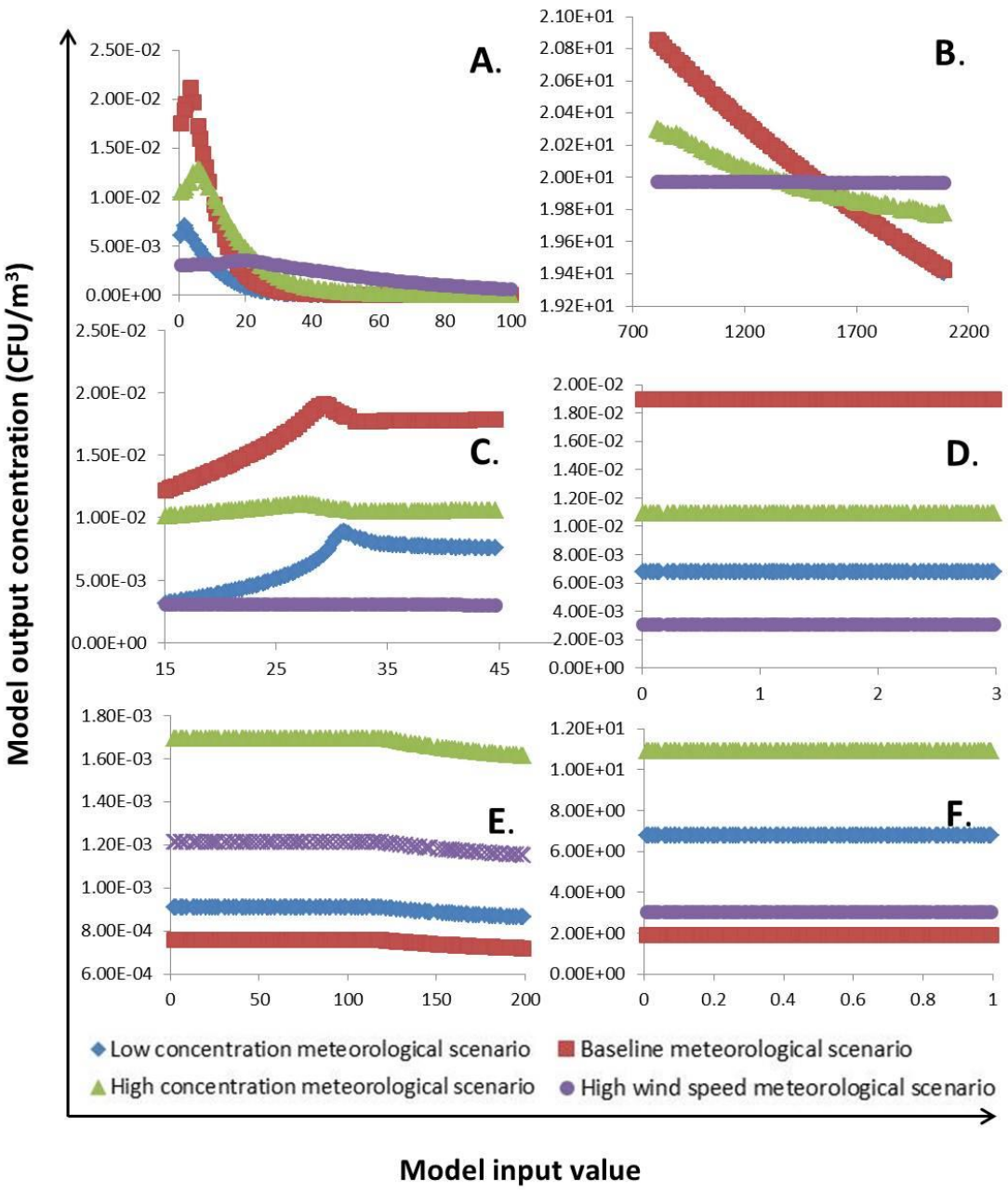

Figure 3-7 OAT changes for the selected model input parameters at 10 metres downwind for A. Pollutant exit velocity, B. Pollutant specific heat capacity, C. Pollutant molecular mass, D. Priestley-Taylor parameter, E. Minimum Monin-Obukhov length, and F. Surface albedo. Please note the differences in the individual graph axis scales.

When observing the gradients of the graphs for all meteorological scenarios at the remaining downwind distances (100, 250, 500, 1000, 5000 and 10000 metres), it was apparent that the data generally followed the same trends of

those presented in Figure 3-7. Therefore this data is not presented. The general trends that were observed are summarised in Figure 3-8.

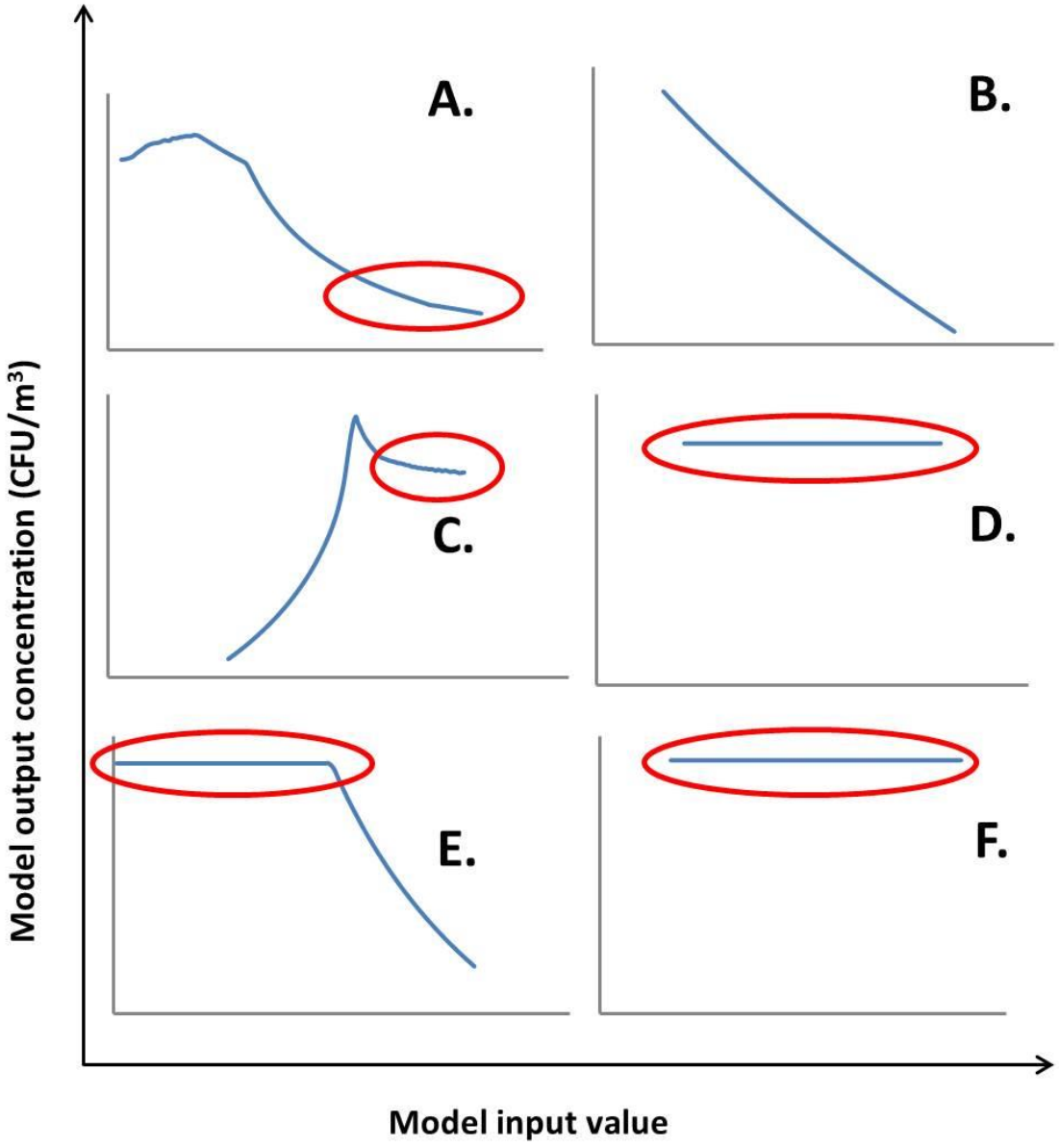

Figure 3-8 General gradient trends for the selected model input parameters for A. Pollutant exit velocity, B. Pollutant specific heat capacity, C. Pollutant molecular mass, D. Priestley-Taylor parameter, E. Minimum Monin-Obukhov length, and F. Surface albedo. Gradients equalling or tending towards zero are highlighted

Flat gradients indicate that a parameter is not sensitive. The gradients in graphs D and F in Figure 3-8 are flat, so these parameters are not sensitive and can be eliminated from the main SA. The gradients of graphs A, C and E are flat or tending towards zero at the points highlighted in Figure 3-8. The gradient in graph B is not flat, and does not show any indication of becoming flat. This indicates that all model inputs within the specified range are sensitive, and thus the full range will be included in the main SA. Table 3-4 lists the parameters and ranges to be included in the main SA, based on the results shown in Figure 3-8.

Table 3-4 Ranges of uncertain parameters to be included in the main SA

Corresponding graph in Figure 3-8	Parameter (Units)	Original range included in the analysis	Range used in the main SA
A	Velocity (m/s)	0-100	0-25
B	Specific Heat Capacity (J/°C/kg)	800-2100	800-2100
C	Molecular mass (g)	15-45	15-45
D	Priestley-Taylor Parameter	0-3	Will not be included
E	Minimum Monin-Obukhov length (m)	1-200	121-200
F	Surface Albedo	0-1	Will not be included

Table 3-4 shows that screening stage 2 has resulted in the exclusion of two parameters, the Priestley-Taylor parameter and surface albedo from the main SA. This reduces the parameter space in which the SA is performed on and hence reduces computational running times. It has also resulted in the range reduction of two of the remaining parameters. The range reduction allows the main SA to be completed at a higher resolution.

3.6 Discussion

The purpose of the screening stages was to reduce the number of input parameters and ranges, and the amount of meteorological data included within the main SA. This is advantageous as it reduces computation running time, the

amount of data to analyse, and data analysis time, whilst increasing the resolution of the main SA. The screening stage was split up into two parts; stage one focussed on meteorological inputs, and stage two on reducing the ranges of selected input parameters. The results from both stages were analysed in a similar way, by observing the general gradient trends on plots of modelled inputs values against modelled output concentrations. There are disadvantages to this method of analysis, which are described below:

- It does not quantify the level of sensitivity of a parameter, only whether an input parameter or parameter range is sensitive or not. For example, it can determine that parameters A and B are sensitive, and that parameter C is not. It cannot determine if parameter A is more sensitive than parameter B
- It is possible to misinterpret some graphs, due to the scaling of the graph axes. For example, if a graph illustrating the range of heights of children aged 10 was plotted on a large range scale, from 0-1000 metres, then it may appear that the height of the school children was constant. In the context of this analysis, an incorrect graph scale may result in the conclusion that a particular input parameter, or input parameter range is not sensitive. When analysing the data in this study, care was taken to ensure that apparent flat gradients were actually flat, by changing the scale of the graphs when necessary, and referring to the raw data.

Despite the disadvantages of this method, it allows large volumes of data to be analysed quickly. A more detailed method of analysis will be used within the main SA, described in the following chapter.

3.6.1 Comparison of results to prior art

As described in section 3.3, SAs have been performed on the ADMS model prior to this study (Mensink and Maes, 1997; Futter, 2000; Harsham and Bennett, 2008; Tamer Vestlund, 2009). However the majority of these studies were completed on input parameters, or input parameter ranges that are not applicable to the open windrow composting scenario. Where possible, the results of screening stages are compared to the findings reported in the

literature. Futter (2000) performed a SA on ADMS version 3, and included meteorological inputs only. This SA was performed in the context of emissions of sulphur dioxide emitted from high stack power stations. Futter observed the effects of altering wind speed, cloud cover, heat flux and boundary layer depth in the dispersion model. Smaller input ranges were included in the study by Futter, when compared to the input ranges included in this study. Futter discovered that all meteorological inputs included in the study were sensitive. This partially agrees with the findings from screening stage 1 presented in this chapter. Wind speed, heat flux and boundary layer depth were all discovered to be sensitive meteorological parameters within this study, which agrees with the results from Futter. However it was found that cloud cover was not sensitive in this study, whereas Futter found that cloud cover was sensitive. These conflicting results may have been caused by modelling at different source heights. It is thought that cloud amount becomes a more important input parameter as stack height increases. To clarify, a source height of 3m was used in this study, based on values previously used within dispersion models when modelling bioaerosol emissions from open windrow composting facilities. Futter used higher source heights of 137-198 metres. Pollutants released during periods of high cloud cover can become trapped, causing elevated pollutant concentrations (Beychok, 1994). Conversely, when pollutants are released above clouds, the layer of clouds can prevent the pollutant from reaching the Earth's surface, significantly reducing the pollutant concentrations at ground level (Oke, 1987; Beychok, 1994). Therefore source height can determine whether a pollutant is released above or below cloud levels, and thus determines whether cloud amount will affect pollutant dispersal. Additionally, low cloud cover scenarios, in other words foggy conditions, cannot be precisely represented within ADMS (Johnson, 2013). As a very low source height was used in this study, and fog conditions cannot be exactly represented within the dispersion model, this explains why cloud cover was not sensitive in this study, whereas Futter, using a higher stack height, found that cloud cover was sensitive.

Tamer Vestlund (2009) performed a SA on ADMS version 3.3 on various model inputs, including meteorological parameters. Tamer Vestlund found wind speed, ambient temperature, and the pollutant exit velocity to be sensitive, and relative humidity to not be sensitive. Mensink and Maes (1997) also found the pollutant exit velocity to be sensitive, agreeing with the results presented in this chapter.

3.6.2 Limitations

By completing the first screening stage, the interaction between meteorological input variables and the remaining model inputs will be limited in the main SA. The main sensitivity analysis will include the most significant meteorological scenarios listed in Table 3-3. This data represents a small proportion of possible meteorological conditions. It was not possible to include all possible meteorological scenarios and inputs within the main SA. However, it should be recognised that it is possible to alter meteorological inputs alongside other model input parameters, but this is technically demanding and time consuming, and thus was not possible within the constraints of this project.

During the second screening stage, interactions between the model inputs were not considered, and parameter alterations were completed OAT. Therefore it is possible that some model inputs appeared to be non-sensitive in the open windrow composting scenario, but in fact were sensitive, in conjunction with another parameter. These interactions are not detectable using an OAT method. Additionally, many assumptions were made regarding the range of the model inputs included. For example, at present there is limited knowledge regarding the pollutant molecular mass of bioaerosols, as explained in Table 3-2. However, all assumptions were justified in an attempt to minimise potential errors.

3.7 Conclusions

Scenario specific sensitivity analysis screening stages were completed to reduce the number of input parameters and ranges included in the main SA. The screening stage was divided into two parts. In both screening stages,

model inputs and ranges relevant to the open windrow composting scenario were used.

Screening stage one was performed on relevant meteorological inputs. It was demonstrated that cloud amount and relative humidity are not sensitive in the open windrow composting scenario, and thus will be excluded in the main SA. Significant gradient changes were observed in the remainder of the meteorological input parameters. It was shown that these significant gradient changes corresponded to certain meteorological scenarios. This reduced the amount of meteorological data to be included in the main SA from over 9000 scenarios to four.

The second screening stage was performed on selected input parameters. It highlighted that the Priestley Taylor parameter and surface albedo were not sensitive, and thus will not be included in the main SA. Of the remaining input parameters, it was shown that some of the variables were sensitive in certain ranges. Therefore only the ranges that were sensitive will be included in the main SA.

By completing the screening stages, the computational running times of the main SA will be significantly reduced. It also reduces the amount of data analysis, and increases the resolution of the main SA.

The next chapter discusses a global SA performed on all parameters within the model. The objective of the SA is to quantify the sensitivity of relevant input parameters within ranges specific to the open windrow composting scenario.

4 Main sensitivity analysis

4.1 Introduction

Sensitivity Analysis [SA] screening stages were performed in the previous chapter, to increase the resolution and decrease the computational running times of the main SA. The first part of the screening stage reduced the numbers of meteorological inputs to be included in the main SA, by identifying the most significant meteorological scenarios. The second part of the screening stage was performed on input parameters in which there is limited knowledge or data, or on input parameters in which the maximum allowed range within the dispersion model was relevant to the open windrow composting scenario. This identified the key ranges to include in the main SA.

This chapter describes a scenario specific main sensitivity analysis performed on the ADMS dispersion model version 4.2. The model input parameters and input parameter ranges included in the SA are representative of bioaerosol releases from open windrow composting facilities. The objective of this chapter is ‘to perform a sensitivity analysis, specific to the scenario of bioaerosol emissions from open windrow composting facilities, to determine which input parameters affect the model output concentrations the most’. This will provide a precedence in which selected input parameter quantification improvements are made. It will also provide an order in which the model input adjustments are made throughout the model calibration. The results from Chapter 3 are utilised in this chapter, which includes:

- A reduced meteorological file consisting of four key dry-weather meteorological scenarios relevant to conditions observed in the UK
- A reduced range of selected model inputs

The majority of previous SA studies using ADMS have been performed using one-at-a-time [OAT] methods, which cannot detect potential parameter interactions (Czitrom, 1999). Therefore potential sensitive interactions are not detected. This SA overcomes this shortcoming by implementing a global sensitivity analysis method. A global sensitivity analysis overcomes the

limitations posed by OAT method by altering all parameters within their specified ranges together (Homma and Saltelli, 1996). Therefore a global SA can be used to determine individual parameter contributions to the overall model output (Saltelli *et al.,* 2000). Global SA methods involve the generation of random numbers inside a plausible parameter input space within a probability distribution for each input parameter (Saltelli *et al.,* 2000; Tomlin, 2013). In basic terms, a probability distribution, sometimes referred to as a probability density function, assigns the probability of an outcome in a random experiment (NIST/SEMATECH, 2012). In a particular scenario, it may have been identified that a particular value of a parameter is more likely within the range of possible inputs. For example, the sum of two standard dice can equal any discrete number between 2 and 12. It is more likely that the sum of the dice will equal 7, as there are more combinations that will result in this value. Thus discrete numbers withinthe range of 2 and 12 can be generated when simulating this example scenario, representing the maximum possible range.. A probability distribution can also be assigned to this parameter to simulate the increased possibility of the sum of the two dice equalling 7. The random numbers generated within the specified ranges and probability distributions are then inputted into the dispersion model, and thus with every model run, each parameter is altered in a random style. There are many techniques for generating these random numbers. The most common methods used in the wider literature include; Monte Carlo simulation [MC] (Saltelli *et al.,* 2004; McLeish, 2005), Latin Hypercube Sampling (McKay *et al.,* 2000; Griensven *et al.,* 2006), High Dimensional Model Representation (Rabitz *et al.,* 1999; Li *et al.,* 2011), and Fourier Amplitude Sensitivity Testing (Helton, 1993; Xu and Gertner, 2011). MC simulation has been the method of choice for many sensitivity analysis studies, including medical studies, among others (Doubilet *et al.,* 1985; Steenland and Greenland, 2004; Balcan *et al.,* 2009), financial modelling (Stambaugh, 1982; Fu and Hu, 1995; McLeish, 2005), chemical modelling (Pandis and Seinfeld, 1989; Campolongo, *et al.,* 1999; Morales-Rodriguez *et al.,* 2012), environmental modelling (Ma *et al.,* 2000; Post *et al.,* 2008; Garcia-Diaz and Gozalvez-Zafrilla 2012). As MC approaches have been adopted for

many years, in several different fields prior to this study, there is a lot of literature surrounding this approach. For these reasons, a MC approach has been adopted in this study.

MC sampling is a method for repeatedly selecting, sometimes referred to as sampling, random numbers within a defined range and probability distribution (Barratt, 2001; Griensven, *et al.,* 2006; Tomlin, 2013). This is completed over and over again, sometimes hundreds or thousands of times, using different random values within the defined distributions. This generates a set of possible outcomes, or values, within the specified ranges and distributions (Vose, 2008; Palisade, 2011). This was completed for every parameter included within the SA as described in section 4.2.

4.2 Method

The main sensitivity analysis was performed on input parameters relevant to this specific scenario, as detailed and justified in Table 4-1. A variance-based global sensitivity analysis was achieved using a MC simulation to evaluate interactions between all inputs. As there is little information regarding the probability of the input values for the model parameters in the composting scenario, a MC method was used to allow input values to be generated over a uniform distribution (Tomlin, 2013), whereby every value across the specified range had an equal likelihood of occurrence (Palisade, 2009). The random numbers generated for each input parameter were produced in the Microsoft® Excel add-in @Risk© (Palisade, 2011). Discrete uniform distributions were also assigned in @Risk©, whereby possible outcomes were specified and each value specified was equally likely to occur (Palisade, 2009), which are required for categorical (for example, ‘on’ or ‘off’) parameters. Random numbers were generated within ranges relevant to this unique scenario as detailed in Table 4-1. Parameters omitted from the analysis, with justification, are also detailed in Table 4-1. Table 4-1 provides the first example of a fully justified set of possible model input parameters relevant to the bioaerosol emissions from open windrow composting facilities scenario. Additional model input files were not considered as they are technically complex to include and many of the options

are applicable to options that are irrelevant to the composting scenario. For example, including options such as the radioactive decay module is not necessary in this analysis, as there is no current evidence to suggest that bioaerosols are radioactive. The efflux options within the model were not included in the SA and were kept at the model default values. This is because the model efflux only alters the units in which the emission is specified (Williams, 2011). Three source types were included within the analysis, point, area and line sources. The justification for the inclusion of these source types is provided in Table 4-1. Due to the technicalities of including different source types, the sensitivity analysis was performed three times, once for each source type. For example, a point source requires slightly different inputs than an area source. Whilst both require a source height input, a point requires a diameter, with coordinates (x, y), whereas an area source requires the geometry for a convex polygon of 3-50 vertices (CERC, 2010b). The model was set-up to give output concentrations at 10, 100, 250, 500, 1000, 5000 and 10000 metres, at a height of 1.7 metres. The distances were chosen to include, and extend beyond, the downwind locations where the sampling equipment was positioned in past studies. A height of 1.7 metres was chosen, as this is the recommended height at which bioaerosols should be sampled according to the sampling protocol (AfOR, 2009). Five hundred random numbers were generated within each input parameter distribution and range. This value was large enough to allow accurate results but small enough so that computational and analysis times were kept to a minimum, as recommended by the software developers, (Palisade, 2009). The random numbers generated by @Risk© were inputted into ADMS, generating 500 separate modelling runs for each source type. Model outputs were produced for every source type, at the selected distances downwind, for every meteorological scenario.

Table 4-1 Sensitivity analysis parameters inclusion, omission and ranges, with justification. N/A denotes 'Not applicable'

Parameter (units)	Included or not?	Justification of inclusion	Range if included	Justification of range
Dry deposition module	Yes	Dry deposition is caused by mechanisms such as gravitational settling, impaction and diffusion (Wesely and Hicks 2000). Bioaerosols are subjected to gravitational settling (Dowd and Maier, 2000; Tamer Vestlund, 2009).	On or Off	N/A
Wet deposition module	Yes	Wet deposition occurs when there is precipitation. Open windrow composting facilities are located outdoors, and are therefore exposed to meteorological conditions.	On or Off	N/A
Radioactive Decay module	No	There is no evidence to suggest that bioaerosols are radioactive and thus this parameter is not included in the SA.	N/A	N/A
Plume visibility module	No	This option only informs the modeller on whether the pollutant plume will be visible or not, depending on the input parameters entered (Lad, 2013), and thus was not included in the main SA.	N/A	N/A
Odours module Chemistry module	No	Although it is recognised that odours and Volatile Organic Compounds [VOCs] are released from composting facilities (Bidlingmaier, 1993; Krzymien and Day, 1997; Yuwano *et al.,* 2003; Müller *et al.,* 2004a; 2004b; Albrecht *et al.,* 2008; Fisher *et al.,* 2008), this project focusses upon bioaerosol emissions from composting facilities and thus this option was not included in the SA.	N/A	N/A

Parameter (units)	Included or not?	Justification of inclusion	Range if included	Justification of range
Buildings module Complex terrain module Coastline module	No	Although composting facilities may be located near to buildings, on complex terrain, or near the coast, these parameters are technically complex to include within the main SA, and are very site specific. Therefore theses parameters are omitted from the main SA. However, if required, the use of these options may be considered during the model calibration and validation stages.	N/A	N/A
Puff module	Yes	Puffs are used when a substance is released over a short period of time. Open windrow composting facilities do not operate continuously, so emissions could be considered as a series of puff emissions. For example, as a long puff emission to respresent the site operational hours, or as multiple shorter puff emissions, to represent individual agitation activities.	On or Off	N/A
Additional model inputs Model outputs	No	These options are technically complex to include and thus were not considered in the main SA. However, if required, the use of these parameters may be considered during the model calibration and validation stages.	N/A	N/A
Pollutant specific heat capacity (J/°C/kg)	Yes	The model default value corresponds to the specific heat capacity of air. The specific heat capacity of bioaerosols has never been quantified before, and thus it is unknown whether the specific heat of bioaerosols will deviate from this value or not.	800-2100	This range was discovered to be sensitive during the second screening stage, as described in section 3.5.2 in Chapter 3.

Parameter (units)	Included or not?	Justification of inclusion	Range if included	Justification of range
Pollutant molecular mass (g)	Yes	The model default value corresponds to the molecular mass of air. As previously described in Table 3-2, the relative genome molecular mass of some bacterial species has been defined (Genthner *et al.,* 1985). However it is unclear what the “mass of one mole” of a bioaerosol component is, and thus has been included in the analysis.	15-45	This range was found to be sensitive during screening stage 2, as described in as described in section 3.5.2 in Chapter 3.
Efflux	No	Efflux only alters the units in which the emission is specified (Williams, 2011) and is therefore not included. This parameter was kept at the model default value.	N/A	N/A
Source type	Yes	Bioaerosol emissions from composting facilities can be represented in the model in various ways. Due to the technical difficulties of including this parameter, the sensitivity analysis will be performed three times, once for each source type included.	Point, Line, and Area only	A jet source is a release where the exit velocity has horizontal and vertical components. Volume sources are assumed not to have any plume rise, for example fugitive emissions from a building (CERC, 2010b). Bioaerosols emitted from open windrow composting facilities are released outdoors and are assumed to have plume rise as conceptualised in Figure 2-4 , so these options are omitted from this study.

Parameter (units)	Included or not?	Justification of inclusion	Range if included	Justification of range
Source height (m)	Yes	Agitation activities result in elevated bioaerosol releases (Taha *et al*, 2006). Agitation activities occur at different heights, depending on the machinery used on-site.	0-5	Agitation activities can take place from ground-level to the maximum height of any machinery used on site. A typical front end loader extends to a maximum height of 4.6 metres (Volvo, 2009) and screening and shredding machinery normally works up to a height of 3.2 metres (Doppstadt, 2009a; 2009b).
Source diameter, L1 or geometry (m)	Yes	As agitation activities result in elevated bioaerosol releases (Taha *et al*, 2006), the geometry of the agitation can vary depending on machinery used, and can be represented in the model in various ways.	0.5-15	The range is based on the areas of compost that can be agitated at any one time. This has been estimated using the technical specifications of the machinery (Volvo, 2009; Doppstadt, 2009a; 2009b).
Pollutant exit velocity (m/s)	Yes	There is very limited data on pollutant exit velocity in this modelling scenario. Therefore at present, it is unknown what range of velocities the pollutant is released at.	0-25	This range was found to be sensitive during screening stage 2, as described in as described in section 3.5.2 in Chapter 3.
Pollutant temperature (°C)	Yes	There is very limited data on the pollutant temperature in this modelling scenario, but it is thought be different to ambient temperature, as explained in section 2.5.3	0-60	This range is based on the core temperature of a composting windrow and the temperature at which the majority of bioaerosols released from composting facilities can survive at (Strom, 1985; Miller, 1996; Sidhu *et al.,* 2001; Swan *et al.,* 2003).

Parameter (units)	Included or not?	Justification of inclusion	Range if included	Justification of range
Emission rate (g/s for a point source, g/m/s for a line source and $g/m^2/s$ for an area source)	No	The emission rate was not altered, and kept at a constant value, of 1g/s, as the sensitivity of this parameter is already known. If the emission rate is doubled, then the output concentration is also doubled (Johnson, 2011a). It should be noted that CFU are not available within the dispersion model, and thus grams are used as a proxy unit.	N/A	N/A
Deposition velocity known Terminal velocity known	Yes	These parameters are associated with the dry and wet deposition options, which are included.	Yes or No	N/A
Deposition velocity (m/s) Terminal velocity (m/s)	Yes	These parameters are associated with the dry and wet deposition options, which are included.	0-10	There is no prior art on deposition or terminal velocities of bioaerosols, and thus the range corresponds to the maximum and minimum values allowed in the model
Particle diameter (m)	Yes	This parameter is associated with the dry and wet deposition options, which are included.	$5x10^{-7}$ – $3x10^{-6}$	Based on the sizes of bioaerosols work estimated by Tamer-Vestlund (2009)
Particle density (kg/m^3)	Yes	This parameter is associated with the dry and wet deposition options, which are included.	1-1100	Has not been quantified for bioaerosols, therefore the range is based on values for air and water (Green and Perry, 2008).

Parameter (units)	Included or not?	Justification of inclusion	Range if included	Justification of range
Conversion factor	No	This parameter only alters the units in which the pollutant output is specified (CERC, 2010b) and thus is not included.	N/A	N/A
Washout coefficient known	No	This parameter can be altered to ‘yes’ or ‘no’ depending on the whether the washout coefficient is known. If the washout coefficient is not known, then the washout is calculated based on precipitation data in the meteorological file (CERC, 2010b). As precipitation data is not included in the meteorological file, this option has been set to ‘yes’ to allow it to be defined within the main model interface.	N/A	N/A
Washout coefficient (/s)	Yes	This parameter is required when the washout coefficient is known.	0-1	There is no prior art on the washout coefficients of bioaerosols, and thus the range corresponds to the maximum and minimum values allowed in the model.
Pollutant type	Yes	This parameter is associated with the dry and wet deposition options, which are included. If the pollutant is modelled as a particle, then the terminal velocity, or particle density and diameter are taken into account (CERC, 2010b)	Gas or Particle	N/A
Duration (s)	Yes	This parameter is associated with the puff option, which is included.	0-36000	The range covers the approximate length of the working hours of a typical operational open windrow composting facility.

Parameter (units)	Included or not?	Justification of inclusion	Range if included	Justification of range
Latitude (°)	Yes	Composting facilities are located at different latitudes.	49.5-58.4	This study is focussing on open windrow composting facilities in the UK. This range covers the latitudes for the British Isles.
Surface roughness (m)	Yes	Composting facilities can be situated on all land types, with differing surface roughnesses.	0.005-1.500	The range correlates to the surface roughness of short grass to urban areas (CERC 2010b).
Minimum Monin-Obukhov length (m)	Yes	This provides a measure of the “stability of the atmosphere” and can differ depending on where the dispersion site is located (CERC 2010a).	121-200	This range was found to be sensitive during screening stage 2, as described in as described in section 3.5.2 in Chapter 3.
Other meteorological parameters	No	Meteorological parameters have already been tested in the first screening stage, asdescribed in sections 3.4.1and 3.5.1. The four meteorological lines presented in Table 3-3 were used in the main SA.	N/A	N/A
Background	No	This main SA is being performed to assess the effects of the modelled inputs on the modelled outputs downwind of a composting facility. Background options are associated with pollutant concentrations upwind of a site, and thus are not considered in the main SA, but will be considered, during the model calibration tests.	N/A	N/A
Grid	No	The grid allows the modeller to define locations at which pollutant concentrations are calculated. Thus it is not a sensitive parameter. The grid will be kept constant throughout the main SA.	N/A	N/A

4.2.1 Data analysis method

The data was analysed similarly to Makler-Pick (2011) using a General Linear Model [GLM]. The GLM was performed using the statistical program Statistica version 11 (Statsoft, 2012). The purpose of a GLM is to explain variability in a dependant variable by a set of categorical or continuous independent variables (StatSoft, 2012). In this application, the dependant and independent variables are the model outputs and inputs respectively. This is an ideal tool for this data as a sensitivity analysis is the study of how model output variation can be apportioned to the variation in the model inputs (Saltelli *et al.,* 2000; Ligmann-Zielinska and Jankowski, 2008; Li *et al.,* 2010). A GLM includes many statistical models including ANOVA, ANCOVA, MANOVA, MANCOVA and linear regression (StatSoft, 2012). A GLM assumes data to be normally distributed (StatSoft, 2013). Assessment of this was made via a normal probability plot of the raw residuals. The normal probability plot showed that the data was not normal so a natural log transformation was completed, and data normality tested again (Crawley, 2007).

A repeated measures analysis of variance [rANOVA] within the GLM observes how the variance of a set of dependant variables is affected by the variance in a set of independent variables (Wheater and Cook, 2000). In this study, the dependant variables are the modelled outputs at the stated distances downwind and the independent variables are the model inputs. If a model input causes a large variation in the model outputs, then that parameter can be considered sensitive. This was tested by observing the p-values for each input parameter. The p-value is an indicator of the statistical significance of a result. If a p-value is low, generally less than 0.05, then the independent variable causes a significant variation in the dependant variable (Hurlbert and Lombardi, 2009; Higgins and Green, 2011; Statistica, 2013). To determine the level of sensitivity of each parameter, a fixed analysis of covariance [ANCOVA] was calculated within the GLM. An ANCOVA combines the characteristics of a rANOVA with regression (Snedecor and Cochran, 1989). Similarly to rANOVA, regressions analyse the relationship of a variable, Y, to another variable X (Snedecor and

Cochran, 1989). To put simply, an ANCOVA also tests the effect of the model inputs on the model output concentrations at various distances downwind. The t-values produced from the ANCOVA indicate whether the gradient of a graph of model input parameters against model output parameters varies from zero or not. The higher the absolute value of t, the more sensitive an input parameter is (Statistica, 2013).

Each input parameter was ranked highest to lowest or most to least sensitive, similarly to Griensven *et al.* (2006), by absolute t-value using standard competition ranking (Winkler, 2012). This was completed for every meteorological scenario, at each distance downwind, for every source type. The ranking information was used to develop sensitivity categories in which to place the model input parameters. The details of the sensitivity categories, and how these relate to the absolute t-value rankings are described below:

- Input parameters were classed as 'very sensitive' if they were ranked between 1 and 10 100% of the time
- If ranked between 1 and 15 100% of the time (but not between 1 and 10 100% of the time) the input parameter was classed as 'slightly sensitive'
- Input parameters were classed as 'not very sensitive' if they were ranked between 1 and 20 100% of the time (but not between 1 and 10 or 1 and 15 100% of the time)
- If the parameter was not ranked between 1 and 20 100% of the time then the input parameter was classed as 'not sensitive at all'

To clarify, if a parameter was ranked between 11 and 15 for 50% of the time but also ranked between 1 and 10 for 50% of the time, then it was classified as 'slightly sensitive'.

When performing the data transformations as described above, it was discovered that many modelled outputs were equal to zero, thus not allowing the data transformation to occur. It was initially thought that, as outputs were calculated at distances as far as 10000 metres downwind of the source, and

that a low emission rate of 1 grams per second was consistently used, that the model could not compute concentrations at very low values. However, after consultation with the model developers, it was made apparent that the model can compute any concentration, high or low (Johnson, 2011c). On closer inspection of the results, it was discovered that the zero values were occurring on the modelled output distances of 500 metres and above, when the wet deposition module was turned on. Therefore, because the wet deposition was turned on, the pollutants were being computationally 'rained out' of the plume, causing zero concentrations at the further distances. Consequently, the data was analysed in two parts. All of the modelled runs that did not include the wet deposition module were analysed separately, using the methods described above. The modelled runs that did use the wet deposition module were carefully observed. All of the downwind distances resulting in zero values were eliminated. These were generally distances between 500 and 10000 metres downwind of the source. The rest of the distances downwind were then analysed as described above, and ranked by t-value.

4.3 Results

As explained in section 4.2, 500 sets of inputs were generated three times for each source type, point, line and area. Outputs were provided at 7 downwind distances of the simulated site, at 10, 100, 250, 500, 1000, 5000 and 10000 metres downwind, for each of the four meteorological scenarios, which are described in Table 3-3. This provided a total of 42000 output values. Modelled inputs were compared to the modelled outputs via a GLM for each meteorological scenario, at each downwind distance, for each source type. These cases were analysed twice, once including all inputs, and once excluding all input runs that used the wet deposition module. This provided a set of 168 cases to analyse using the GLM. This is conceptualised in Figure 4-1.

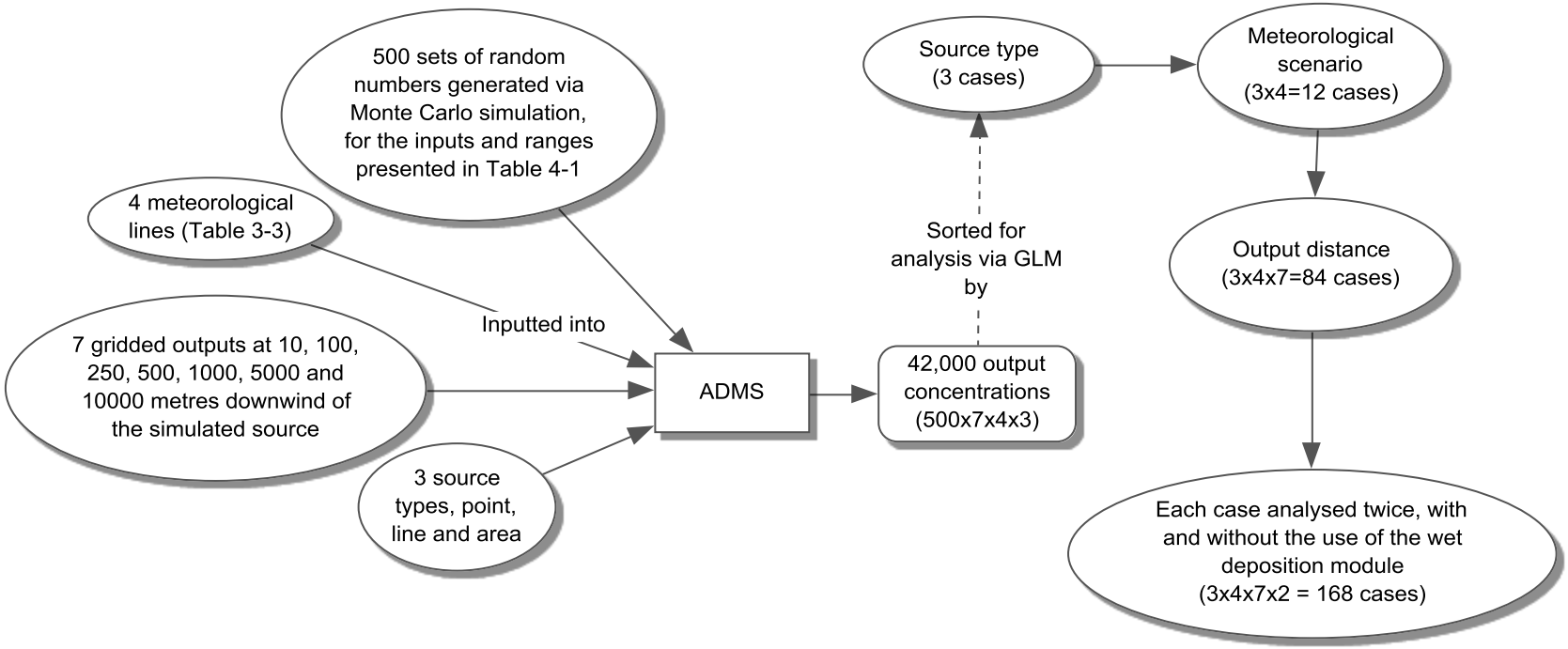

Figure 4-1 Conceptualisation of how the SA was completed, and how the results were grouped for analysis via a GLM

As described in section 4.2.1, each input parameter for each case was ranked by absolute t-value. This information was used to sort the model input parameters into sensitivity categories, as described in section 4.2.1.

As 168 cases were analysed, the process of how each case was ranked and used to sort the model input parameters into sensitivity categories is not presented. However, the results from three of the 168 cases is presented and described in this section. The sensitivity categories developed through ranking the model inputs indicates which input parameters affect the modelled outputs the most, in the context of bioaerosol emissions from open windrow composting facilities. Table 4-2 provides the absolute t-value for each input parameter for the three cases, with rankings from highest to lowest t-value, or in other words, from most sensitive to least sensitive. The three cases presented were generated when modelling as an area source, considering all inputs, including the wet deposition module, at 100 metres downwind. Case 1 was generated when the lowest concentration meteorological scenario was used and cases 2 and 3 when the highest concentration and high wind speed meteorological scenarios were used respectively. The meteorological scenarios used are detailed in Table 3-3.

Table 4-2 Absolute t-values generated through completing a GLM, and rankings for each model input parameter based on the absolute t-value for three of 168 analysis cases. Each absolute t-value has been rounded to two decimal places. Red values indicate a significant p-value (<0.05)

Model input parameter	Case 1		Case 2		Case 3	
	Absolute t-value	Ranking based on t-value	Absolute t-value	Ranking based on t-value	Absolute t-value	Ranking based on t-value
Pollutant exit velocity	9.38	1	7.60	1	2.89	9
Pollutant molecular mass	6.78	2	5.80	3	1.62	11
Wet deposition module	5.66	3	7.03	2	5.43	6
Minimum Monin-Obukhov length	3.90	4	2.09	12	0.79	16
Horizontal source geometry	3.80	5	2.45	7	5.43	4
Vertical source geometry	2.55	6	2.39	8	5.65	3
Pollutant temperature	2.54	7	1.59	15	1.51	13
Dry deposition module	2.46	8	2.32	9	5.49	5
Deposition velocity known (for a particle)	2.23	9	2.92	5	0.96	14
Surface roughness	1.60	10	1.89	13	2.50	10
Source height	1.48	11	1.67	14	1.60	12
Particle diameter	1.28	12	0.18	22	0.48	18
Latitude	1.21	13	0.89	18	0.41	19
Terminal velocity known	1.00	14	2.65	6	6.31	1

Model input parameter	Case 1		Case 2		Case 3	
	Absolute t-value	Ranking based on t-value	Absolute t-value	Ranking based on t-value	Absolute t-value	Ranking based on t-value
Pollutant type	0.87	15	2.93	4	5.86	2
Terminal velocity	0.64	16	0.28	21	0.39	20
Washout coefficient	0.45	17	1.89	13	3.66	8
Pollutant specific heat capacity	0.30	18	0.44	19	0.77	17
Deposition velocity known (for a gas)	0.29	19	2.26	11	4.15	7
Particle density	0.06	20	1.47	16	0.35	21
Deposition velocity (for a particle)	0.05	21	2.29	10	0.92	15
Deposition velocity (for a gas)	0.04	22	0.29	20	0.16	22

Section 4.2.1 described how the absolute t-value rankings were used to develop sensitivity categories.

Table 4-2 shows that the wet and dry deposition modules, the pollutant exit velocity, and vertical and horizontal source geometries were consistently ranked in the top 10 in all three cases. These input parameters were ranked between 1 and 10 in all 168 cases. From these results, these input parameters were classed as ‘very sensitive’ when modelling with an area source type. Similarly, the pollutant molecular mass was ranked at 2, 3 and 11 in the three cases presented in Table 4-2. This parameter was ranked between 1 and 15 100% of the timein the 168 cases analysed. Therefore this parameter was classed as ‘slightly sensitive’. The rankings for each input parameter for all 168 cases were analysed in this way, allowing the input parameters to be categorised by level of sensitivity. The overall results are presented in Table 4-3.

Table 4-3 Sensitivity categories, developed by ranking the absolute t-value

Sensitivity Category	Source type		
	Point	**Area**	**Line**
Very Sensitive	Wet deposition module Pollutant molecular mass Dry deposition module Source diameter Pollutant exit velocity	Wet deposition module Horizontal source geometry Vertical source geometry Dry deposition module Pollutant exit velocity	Horizontal source geometry Vertical source geometry Wet deposition module Pollutant exit velocity Dry deposition module
Slightly sensitive	Surface roughness Source height Pollutant temperature Washout coefficient Pollutant type Deposition velocity known (for a particle) Deposition velocity known (for a gas) Terminal velocity known	Surface roughness Source height Pollutant temperature Pollutant molecular mass Pollutant type Deposition velocity known (for a particle) Terminal velocity known	Surface roughness Source height Pollutant molecular mass Pollutant temperature Washout coefficient Pollutant type Deposition velocity known (for a particle) Deposition velocity known (for a gas) Terminal velocity known
Not very sensitive	Minimum Monin-Obukhov Length Pollutant specific heat capacity Deposition velocity (for a gas) Particle density Terminal velocity Deposition velocity (for a particle) Particle diameter	Washout coefficient Deposition velocity known (for a gas) Minimum Monin-Obukhov Length Pollutant specific heat capacity Particle density Terminal velocity Deposition velocity (for a particle) Particle diameter Latitude	Minimum Monin-Obukhov Length Pollutant specific heat capacity Latitude Particle density Terminal velocity Particle diameter
Not sensitive at all	Puff module Duration Latitude	Deposition velocity (for a gas)	Deposition velocity (for a particle) Deposition velocity (for a gas)

4.4 Discussion

4.4.1 General observations of the sensitive parameters

- The majority of the sensitive model input parameters are associated with the emission source.

When observing the simple Gaussian model equation, Equation 2-1 in Chapter 2 (Keddie, 1980; Essa et al., 2003), it is apparent that the equation is driven by certain source parameters including the pollutant emission rate and the height of the emission. The conditions at the source determine initial plume size, rise and location, and thus it is unsurprising that the source input parameters contribute to large variation in the modelled output concentrations.

It was expected that the pollutant exit velocity would have a large effect on the output concentration, as this parameter determines the vertical velocity of the pollutants at the source exit (CERC, 2010b). At higher exit velocities, the pollutant plume is less affected by the effects of ambient wind speeds, reducing the levels of plume curvature into the horizontal plane (Beychok, 1994), thus impacting pollutant concentrations.

The pollutant temperature, alongside meteorological factors such as ambient temperature, determines the amount of plume rise (De Nevers, 2000), and thus the pollutant concentrations observed at ground-level. ADMS is capable of processing the effects of plume rise (Robins *et al.,* 2009), and thus it was expected that this parameter would be sensitive within the dispersion model. Similarly the physical height of the source affects the pollutant concentrations observed at ground-level (De Nevers, 2000), and thus it was expected that this input parameter would also be sensitive. Additionally, the source geometry, vertical and horizontal or the diameter of the source, also has an effect on plume rise, and also plume spread (Ministry for the Environment, 2004; CERC, 2012b), and thus was expected to be sensitive.

- The wet and dry deposition modules were sensitive.

It was expected that the wet and dry deposition module would be sensitive within the dispersion model. The dry deposition module simulates the effects of

pollutant loss from the plume due to diffusion and gravitational settling (CERC, 2010b). Similarly, the wet deposition module models the effect of precipitation on pollutant 'wash out' from the plume (CERC, 2010b). Therefore it is unsurprising that these options were discovered to be sensitive and had a large effect on the modelled output concentrations.

- The meteorological parameters included within the main SA are not very sensitive, with the exception of surface roughness

Surface roughness is a parameter which simulates the effects of turbidity and thus atmospheric stability (Oke, 1987). Therefore it was anticipated that the surface roughness would be a sensitive input parameter, as a higher surface roughness results in a more turbulent atmosphere immediately above the Earth's surface (Oke, 1987; EPA, 2005), which consequently provides more atmospheric mixing and thus pollutant dispersal (Oke, 1987). The minimum Monin-Obukhov length [MMOL] and latitude were not very sensitive, if at all within this scenario specific SA. The MMOL provides a measure of the atmospheric stability, based on residential heat generation (CERC, 2010b), as discussed in the previous chapter. As MMOL effectively simulates the consequences of atmospheric stability, it was expected that the MMOL would be more sensitive than the results indicate. However, this SA has been performed on specific ranges, relevant to the open windrow composting scenario, and thus it may be more effective when other selected parameters are altered.

The latitude is used within the meteorological processor to calculate the incoming solar radiation (Johnson, 2011b; Thomson, 2012). Solar radiation affects the amount of heat energy in the atmosphere, which modifies the thickness of the boundary layer (Oke, 1987; Johnson, 2011b). Latitudinal effects are more important nearer to the equator, where there are increased levels of solar radiation (Johnson, 2011b). As this study and SA has focussed on composting in the UK, and thus a very small range of latitudinal values, it was predictable that latitude would not have a large affect the modelled output concentration.

- The puff module, and parameters associated with the puff module, are not sensitive

All inputs related to the puff module were observed to be not sensitive in this modelling scenario. The puff was incorporated into the SA by modelling the puff as a time integrated (dose) instead of a time dependant puff. This seemed the most appropriate option as the time-integrated (dose) option calculates the total quantity of the pollutant at the receptor location, from first to last exposure (CERC, 2010b). However, when the model calculates the puff spread and mean concentrations for a time-integrated (dose), it uses the same equation as a continuous release with an equivalent release rate (CERC, 2012b). Puff type calculates the output concentration using the same equation as a non-puff release. This seems to be the most reasonable explanation as to why the puff module appears to be non-sensitive. In retrospect, the time dependant puff option should have been used in the main SA. The results are therefore inconclusive and require further investigation.

- The majority of categorical parameters are sensitive

The categorical parameters determine what options and calculations are made within the dispersion model, and thus it was predicted that these parameters would contribute to large variations in the model output concentration. For example, there is an option within the model that determines whether the terminal velocity of a particle is known. The terminal velocity accounts for the material lost from the plume due to gravitational settling (Apsley and CERC, 2012). This option can only be altered if the categorical input ‘pollutant type’ is set as a particle (CERC, 2010b). To allow particles to be modelled, the dry deposition module should be used (Johnson, 2011b). If the terminal velocity is known, then gravitational settling within the plume is calculated using the terminal velocity input parameter. If the terminal velocity is not known, then gravitational settling within the plume is calculated using the particle diameter and density inputs (CERC, 2010b; Apsley and CERC, 2012).

4.4.2 Limitations

Although this chapter presents the first SA performed on input parameters and ranges specific to the open windrow composting scenario, there are still many limitations to this work. The limitations associated with the screening stages of the SA, as discussed in section 3.6.2, were also carried over to the main SA.

One of the most major limitations of the SA is associated with the parameters and parameter ranges included in the SA. There is very limited information regarding what ranges are relevant to this specific scenario for several model input parameters. Therefore there is some reservation regarding whether parameter ranges specific to the open windrow composting scenario have been included within the main SA. Similarly, due to a lack of information, uniform distributions were assigned to every input parameter range when generating random inputs to include within the SA. This may have reduced the resolution of the SA, by including inputs, or combinations of inputs that are not feasible in the open windrow composting scenario. Despite these limitations, the ranges included were considered carefully, attempting to include every feasible value for this specific scenario.

The Monte Carlo method used to generate the random input values used within the SA has been criticised for being an “approximate technique” (Vose, 2008). Additionally, it has been reported that Monte Carlo simulations can lead to ambiguous results if incorrect or unsuitable ranges are included (Ibbotson Associates, 2005). Therefore it may have been more suitable to use a different random number sampling technique, such as Latin Hypercube Sampling (McKay *et al.,* 2000; Griensven *et al.,* 2006). However, this method was chosen as it has been widely used in many studies in many different research fields, and was suitable for this initial SA.

Another limitation of this study is associated with the meteorological inputs. Due to model technicalities, it was computationally more time effective to evaluate the majority meteorological input parameter separately, as a screening stage, as discussed in the previous chapter. Therefore, although different

meteorological scenarios were modelled, it is possible that some model interactions were overlooked.

4.4.3 Implications of work

The SA has determined which model inputs influence the modelled outputs the most, thus providing precedence to model input parameter quantification improvements, which are presented in Chapter 7. Without the completion of the SA, quantification of non-sensitive parameters may have been completed. Therefore by completing this SA it is likely that sampling times and cost have been reduced, by by preventing unnecessary parameter quantifications. For example, pollutant particle diameter was extensively measured by Tamer Vestlund (2009) which was very costly and time consuming. However, the pollutant particle diameter is not very sensitive, and thus quantification of this parameter may have been unnecessary for improved modelling. Additionally, the knowledge acquired from the SA can be applied to the model calibration test, providing priority on model input adjustments, as presented in Chapter 5. For example, the most sensitive parameters can be adjusted within justified ranges initially, as these inputs affect the modelled outputs the most. The results from this SA can also be used to provide a set of initial model inputs in which model input adjustments can be made.

4.5 Conclusions

A SA performed on inputs and ranges relevant to the open windrow composting scenario was completed on ADMS for the first time, to understand which model input parameters affect the model output parameters the most. Results were analysed using a GLM, which explained the variability in the model output concentrations by apportioning the results to the model input parameters. It was discovered that:

- The majority of the sensitive model input parameters are associated with the emission source
- The dry and wet deposition modules were sensitive

- The meteorological parameters included within the main SA, except surface roughness are not very sensitive
- The puff module, and parameters associated with the puff module, are not sensitive
- The majority of categorical parameters are sensitive

The completion of this SA has provided an improved understanding of how the ADMS dispersion model performs when applied to the open windrow composting scenario. The results of the SA can be used to:

- Provide precedence to model input parameter quantification improvements (Chapter 7)
- Specify which model input parameters are adjusted initially when calibrating the model within the open windrow composting scenario (Chapter 5)

The next chapter discusses the model calibration completed on the ADMS model for this unique scenario. The purpose of a model calibration is to adjust model inputs until the modelled output concentrations correspond to a set of sampled data set. The information acquired from this chapter will be used to determine the order of model adjustments, with the more sensitive model input parameters being adjusted initially.

5 Model calibration

5.1 Introduction

A Sensitivity Analysis [SA] was performed on ADMS version 4.2, to determine the input parameters that affect the model outputs the greatest in the composting scenario, as discussed in Chapter 4. This information can be used to perform a scenario specific model calibration. A model calibration is the process of modifying the model input parameters, within an acceptable range or criteria, until the model outputs fit to a set of measured data (Sahraoui and Jayakrishnan, 2005). Model calibration is necessary to assess whether model predictions are rational in comparison to reality. The parameter sensitivity information, which was achieved in Chapter 4, can be applied to the model calibration, as the most sensitive model inputs can be modified first.

Confidence in model outputs, when applying the model to the open windrow composting scenario, is vital so that the model can be used to predict bioaerosol concentrations where current sampling methods are impractical or impossible to use. For example, using a dispersion model to estimate bioaerosol concentrations over wider spatial and longer temporal scales would provide a more detailed insight into bioaerosol exposure at the nearest sensitive receptors. Similarly, confidence in the modelled outputs, when simulating bioaerosol emissions from the open windrow composting scenario, can allow emissions from a proposed facility to be estimated, aiding with the site planning and permitting processes. However, at present, only modest progress has been made when using the ADMS model to predict bioaerosol emissions from composting facilities (Taha *et al.,* 2006; 2007, Drew *et al.,* 2007). Additionally, there have been no model calibrations, for any type of dispersion model, when simulating bioaerosol emissions from open windrow composting facilities. Therefore this chapter describes the first scenario specific calibration when using the ADMS dispersion model.

5.2 Data overview

The data used within the calibration was collected by Pankhurst (2010) from Lount organic waste composting, an open windrow composting facility located in Leicestershire, UK. This facility is now referred to as Lount. This dataset is one of the two most extensive datasets available in the UK for the open windrow composting scenario. The second dataset, collected from a different composting facility, is used throughout the model validation (chapter 6), which is described in the following chapter, in section 6.2.

Lount is an open windrow composting facility located near to Ashby-de-la-Zouch in Leicestershire. The site is located in-between two major roads, the B587, located to the north west, and the A42, located to the south east. Lount processes mainly green-waste compost and is situated on a capped landfill. The site is relatively flat, with an incline of 4% from north-east to south-west, and is situated in a rural agricultural area, with some small areas of woodland surrounding to the west and east of the site (Golder Associates, 1998; Pankhurst, 2010).

Bioaerosols were collected in triplicate using SKC personal filter samplers, as detailed in the bioaerosols sampling protocol, (AfOR, 2009). Sampling locations were logged using a Global Positioning System [GPS] and site activities were recorded using a video camera on-site. Samples were duplicated in the laboratory. *Aspergillus fumigatus,* actinomycetes, Gram-negative Bacteria, and endotoxins were analysed for the majority of sampling locations. As samples were taken in triplicate in the field, and duplicated in the laboratory, the mean average of the sample replicates were used to compare the sampled data to the model outputs. It is recommended that the mean average of parallel samples is presented in the sampling protocol (AfOR, 2009). As a mean average of the sampled data was used, the standard error of the mean [SEM] of the sampled data is provided wherever possible. The Lower Limit of Detection [LLOD] for this sampling method was 757 CFU/m^3 (Pankhurst, 2010), therefore a ‘zero’ value could represent a bioaerosol measurement of 0-756 CFU/m^3. Consequently, to represent a ‘worst-case scenario’, all ‘zero’ values were altered to 756 CFU/m^3.

Aspergillus fumigatus concentrations only were compared to the modelled outputs because:

- It is the most consistent pollutant, for example, it appears consistently for every sampling location in every dataset available
- There is more information published on *Aspergillus fumigatus*
- It has important health implications (Nadal *et al.,* 2009; Environment Agency, 2010; Vilavert *et al.,* 2012)

The sampling data was collected over 15 separate site visits taken between the 27th of September 2007 and the 30th of July 2008. The sampling strategies used to collect the data altered depending on the purpose of the site visit, as detailed in Pankhurst (2010), and summarised below:

- A 'traditional' sampling method was used, whereby the AfOR protocol was mostly followed. This included taking one sample at upwind of activities on the site, two or three samples on site during periods of agitation activities, and non-activity, and downwind of the site, at 50, 100 and 150 metres
- Transect sampling strategy, where samples were taken at regular intervals down and upwind of site on a single transect which was determined by the wind direction. This initially involved taking at least two samples upwind, on-site and downwind. However, when results showed that the bioaerosols were not being detected on several of the upwind measurement, this was modified to include more downwind samples, up to 280 metres downwind of the site
- A strategy designed to capture episodic releases was also adopted, whereby two samples on-site or downwind of the site were taken simultaneously. This was completed up to 300 metres downwind of the site

Overall, despite which sampling strategy was used the sampled data can always be categorised into one of three categories; data collected at locations upwind of the site, downwind of the site or on-site. Modelled outputs were compared to sampled data downwind of the facility only throughout the model

calibration. This is because it is desirable to have a calibrated model that can be used to predict exposure downwind of the composting facility, particularly at sensitive receptors.

5.3 Approach

The calibration was split into two stages. Stage one was completed to provide an initial set of inputs with which to commence the calibration, utilising the data acquired during the sensitivity analysis. Stage two involved modifying these initial input parameters, one-at-a-time within justified ranges to determine the best fit between the model outputs and the sampled data. These stages are described in more detail in sections 5.3.1 and 5.3.2 respectively.

5.3.1 Calibration stage 1

Modelled output concentrations from the SA were compared with sampled concentrations via a means with error plot in Statistica 11 (© StatSoft, Inc. 1984-2012). SA outputs for every source type (point, line and area) and meteorological scenario were combined and compared to sampled data at 10, 100 and 250 metres downwind of the source. These distances were chosen as they were present in both the SA output data, as modelled output distances, and in the measured data. A means with error plot of the sampled data was drawn for each distance downwind, with a 95%confidence interval. The modelled output data was overlaid via a scatter plot for each of the source types to indicate which modelled outputs corresponded to the measured data. The median input values of any model outputs that fell within a 95% confidence interval of the measured data were used as initial model input values for calibration stage 2.

5.3.2 Calibration stage 2

The overall approach of calibration stage 2 was partly based on the methodology developed by Nash and Sutcliffe (1970) for river flow forecast modelling. A summary of the approach used in this chapter is illustrated in Figure 5-1.

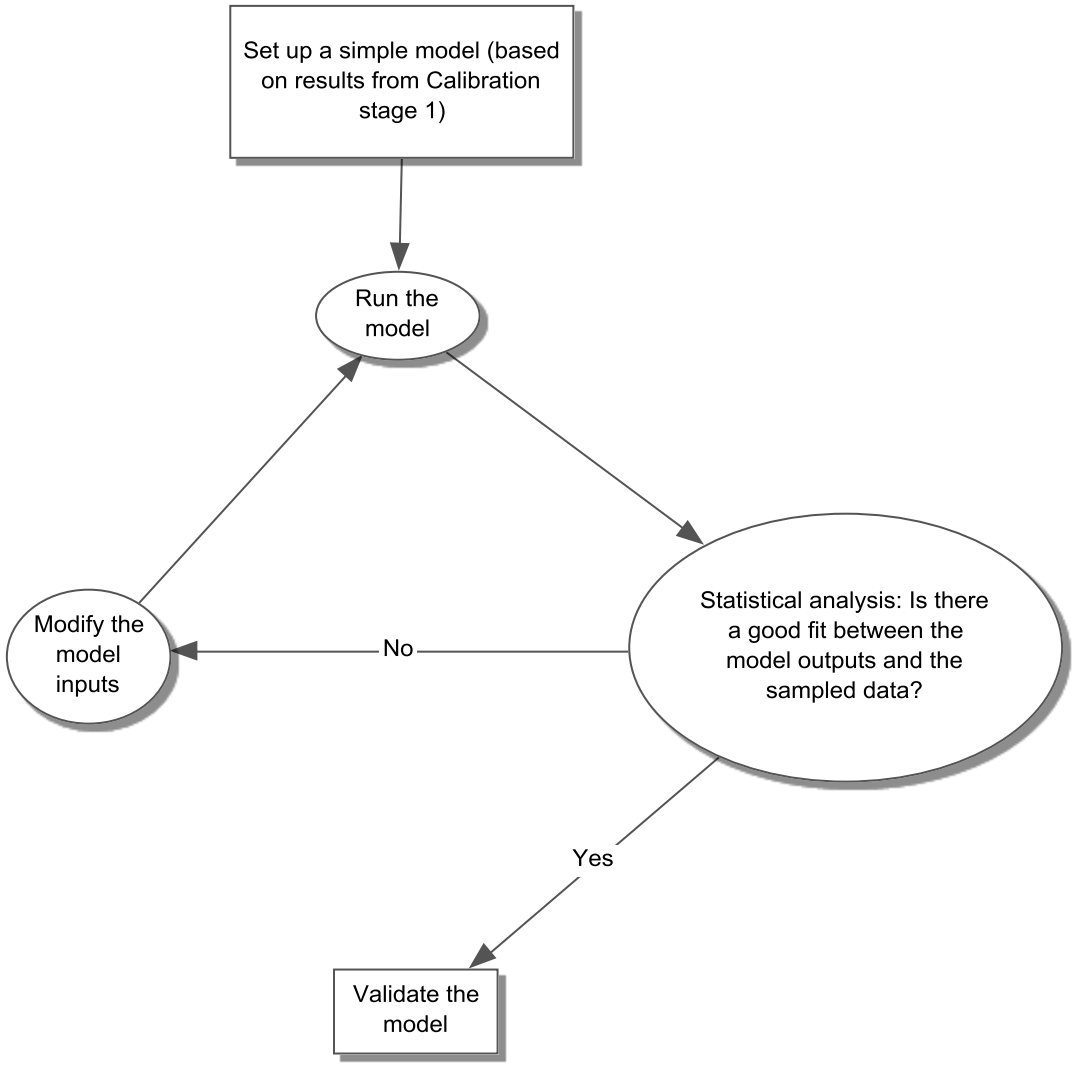

Figure 5-1 Overall schematic of the method used for stage 2 of the calibration (based on a methodology developed by Nash and Sutcliffe (1970))

Initial model inputs were created based on the information gained in calibration stage 1, as described in sections 5.3.1 and 5.4.1. The initial model inputs were set-up as simply as possible, as modifications were likely to become increasingly complex. A calibrated and validated model with simple model inputs is more desirable when using the model for regulatory purposes, as it would be easier and quicker to set-up and run, and would therefore be more cost effective to operate, as it would require minimal sampling data. Therefore the model was set up with one line of meteorological data, based upon the results of calibration stage 1, to provide uniform weather conditions across the modelled site. As modelled weather conditions were uniform, a simple grid was

used to provide modelled outputs at the sampled distances downwind for direct comparison with the sampled data. This is conceptualised in Figure 5-2.

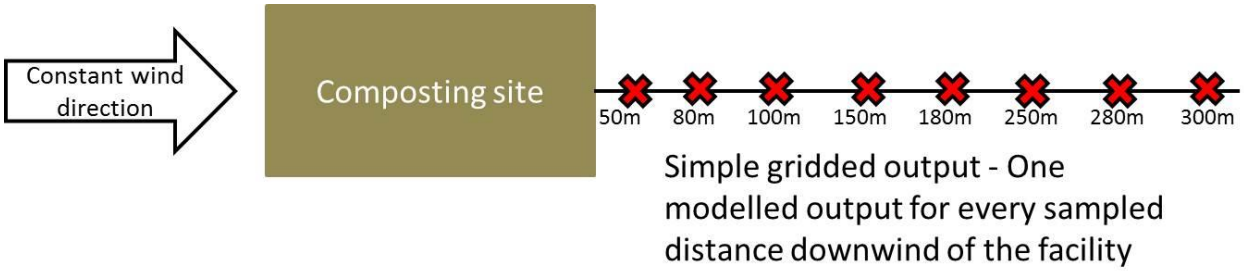

Figure 5-2 Conceptualisation of the simple gridded outputs used in the initial model runs of calibration stage 2 (not to scale)

Figure 5-2 shows that by initially using a simple model set-up, only one modelled output concentration is provided for each sampled distance downwind, irrespective of how many measurements were taken at that location. For example, four measurements were taken at 50 metres downwind of the facility, on different sampling occasions. These measurements were, initially, compared to one modelled output at the corresponding distance downwind, when the simple model set-up was used.

The goodness of fit between the model outputs and the sampled data was determined statistically, as described in section 5.3.3. Parameter modifications were made one-at-a-time [OAT] from the initial model inputs provided from calibration stage 1. Modifications were made OAT to fully understand the effects of the model inputs on the model outputs. The inputs were modified in order of sensitivity, and within ranges applicable to the open windrow composting scenario, as described in Table 4-1 in Chapter 4. The current level of information for each model input parameter varies. For example, source geometry can be easily estimated or measured, whereas the specific heat capacity of *Aspergillus fumigatus* cannot. Therefore, the model parameters were altered in order of information level, from inputs with the most information or data or confidence for the open windrow composting scenario to the least. A colour code was applied to the model inputs to allow rapid distinction between

the levels of information between each parameter. The colour codes applied are described below:

- Green was used if there was existing measured or estimated data for that parameter, with clear information regarding how the parameter was measured or estimated for the parameter, in the context of the open windrow composting scenario.
- If there was existing data on that parameter, for the open windrow composting scenario, but it is not clear how the data was measured, estimated or justified, then the parameter was colour coded orange
- Categorical parameters were not colour coded
- All other parameters were colour coded red

It should be noted that if a parameter is colour coded green, indicating that there is existing measured or existing data for that parameter, it does not necessarily mean that the parameter has been fully quantified in the open windrow composting scenario, and it may be possible to improve the quantification of the parameter.

Table 5-1 shows this colour code applied to the sensitivity categories, originally presented in Table 4-3.

Table 5-1 Sensitivity categories, originally presented in Table 4-3, with colour coding, to represent current levels of information for that parameter, within the context of the open windrow composting scenario.

Sensitivity Category	Source type		
	Point	**Area**	**Line**
Very Sensitive	Wet deposition module Pollutant molecular mass Dry deposition module Source diameter Pollutant exit velocity	Wet deposition module Horizontal source geometry Vertical source geometry Dry deposition module Pollutant exit velocity	Horizontal source geometry Vertical source geometry Wet deposition module Pollutant exit velocity Dry deposition module
Slightly sensitive	Surface roughness Source height Pollutant temperature Washout coefficient Pollutant type Deposition velocity known (for a particle) Deposition velocity known (for a gas) Terminal velocity known	Surface roughness Source height Pollutant temperature Pollutant molecular mass Washout coefficient Pollutant type Deposition velocity known (for a particle) Deposition velocity known (for a gas) Terminal velocity known	Surface roughness Source height Pollutant molecular mass Pollutant temperature Washout coefficient Pollutant type Deposition velocity known (for a particle) Deposition velocity known (for a gas) Terminal velocity known
Not very sensitive	Minimum Monin-Obukhov Length Pollutant specific heat capacity Deposition velocity (for a gas) Particle density Terminal velocity Deposition velocity (for a particle) Particle diameter	Minimum Monin-Obukhov Length Pollutant specific heat capacity Particle density Terminal velocity Deposition velocity (for a particle) Particle diameter	Minimum Monin-Obukhov Length Pollutant specific heat capacity Latitude Particle density Terminal velocity Particle diameter
Not sensitive at all	Puff module Duration Latitude	Deposition velocity (for a gas) Latitude	Deposition velocity (for a particle) Deposition velocity (for a gas)

To summarise, the parameters were modified according to the level of sensitivity and level of information in the open windrow composting contest. A schematic depicting the order of modifications is provided in Figure 5-3.

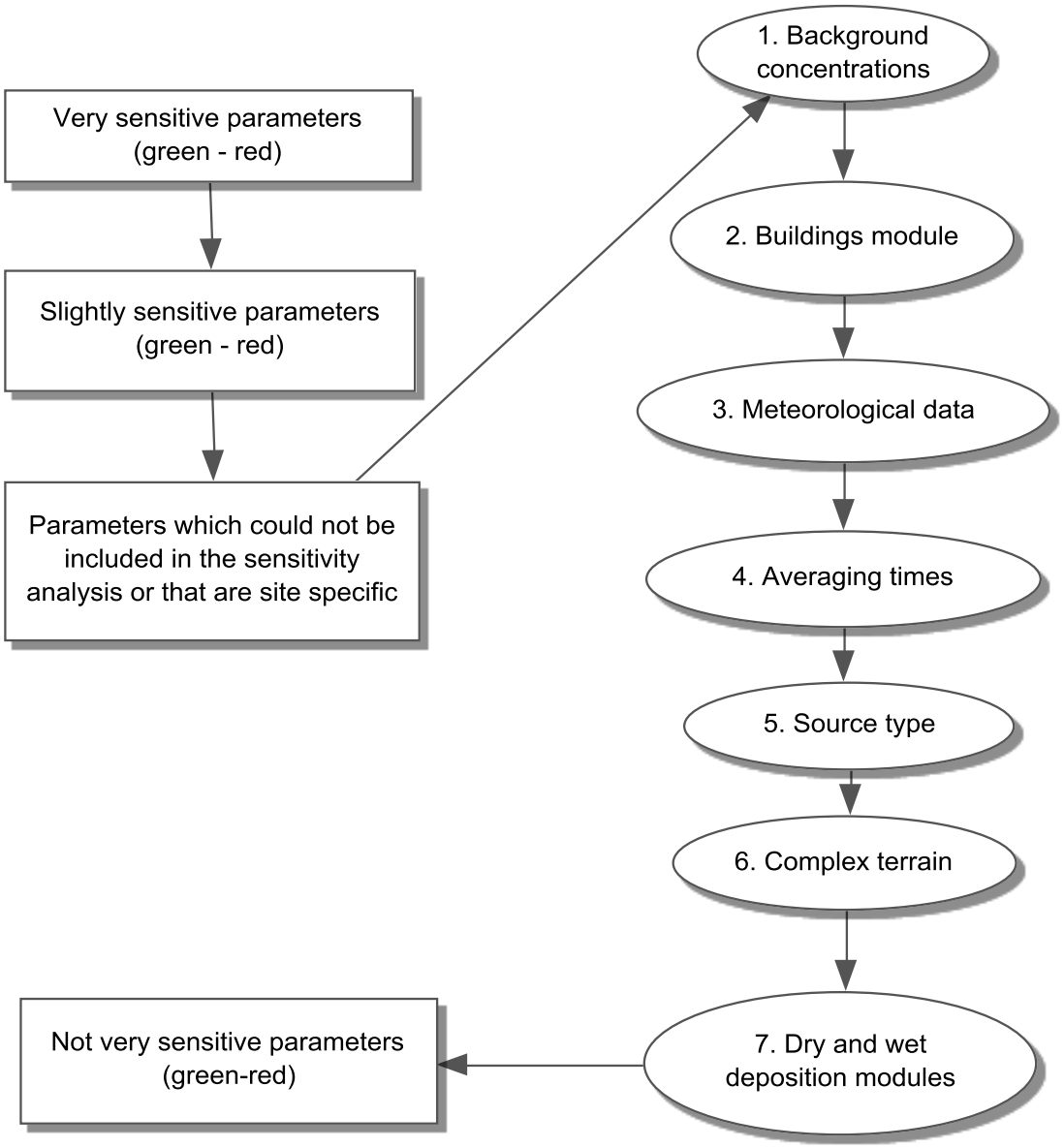

Figure 5-3 Order of modifications in the calibration, based on parameter sensitivity and level of existing knowledge

As shown in Figure 5-3, the order of possible model input modifications were planned in full. However if the statistical analysis showed that correspondence between the model outputs and the sampled data had been achieved prior to

the end of this schematic, then the calibration stage was halted, as depicted in Figure 5-1.

The ‘very sensitive parameters’ were altered first, followed by the ‘slightly sensitive parameters’ as these parameters alter the model outputs parameters the greatest for this specific scenario. The order of the sensitive parameter alterations was determined by the level of information on that parameter in the open windrow composting context, indicated by the colour coding. Parameters with the most data or knowledge (green) were altered first, as more informed decisions could be made when altering these parameters to give an optimal output. Complex input parameters, such as the wet and dry deposition modules and their associated model inputs, were not altered at this stage as a simple calibrated model is more desirable, as explained previously.

Site specific parameters, and parameters not included in the SA were then modified. The order of modification was determined by the complexity of the parameter and the amount of data and information known about the parameter. The least complex parameters with data or knowledge available were altered first. The order of parameter alterations is detailed and justified below:

1. Background option

   The background option allows the model user to input any background concentrations of a pollutant (CERC, 2010b). This option is easy to use and adjust within ADMS. Data should be widely available as background, or ‘upwind’, values are required when sampling bioaerosols (AfOR, 2009)
2. Buildings option

   The buildings option simulates the effects of buildings on pollutant dispersal, primarily accounting for the effects of entrainment in the cavity region of a building (CERC, 2010b). More information is required to use this option than the background option, but the information needed can be easily measured on-site or estimated using measuring tools on geographical information programs such as ArcMap™ (Esri®, 2012) and Google Earth™, (Google©, 2012)
3. Meteorological data

Meteorological data is more complex to include when compared to the buildings module, but data is readily available. Officially, meteorological conditions should be monitored thoroughly on the sampling day (AfOR, 2009). However this has not always been achievable, particularly on older data sets, before this requirement was regimented. Nevertheless past meteorological conditions can be purchased from the UK Meteorological Office© (Met Office, 2011). Purchased meteorological data is readily available and of good quality and high resolution (measurements every hour), and thus this option is explored prior to modelling with sampled meteorological data. Occasionally additional inputs related to the meteorological data such as the 'calms' option are required, and were included if necessary.

4. Averaging times

   Averaging times represent the average concentrations of a pollutant over a specified time scale (for example, over 1 hour) (CERC, 2010b). Averaging times are easily altered within the model, but there is no current guidance to indicate what value should be used when modelling bioaerosols in the open windrow composting context

5. Source type

   Different source types can be used depending on the scenario that is simulated. Point, jet, line, area and volume sources can be modelled within ADMS (CERC, 2010b). Multiple source types can be used to represent different agitation activities, which can be 'turned on' or 'turned off' using the time-varying source options.Alternatively, emissions can be represented simply as a single continuous source. A simple singular source will be tested first, abd if necessary more complex options will be used.

6. Complex terrain option

   The complex terrain option allows the modeller to simulate pollutant dispersal in areas where there is complex topography, for example, where the gradient exceeds 1:10 (CERC, 2010b). This option is difficult to include in the model and expensive data may need to be purchased

7. Wet and dry deposition options

   The wet and dry deposition options account for loss of material in the pollutant plume, for example, due to the effects of gravitational settling or washout. The wet and dry deposition modules are complex to include as they involve altering many other parameters related to these modules. There is little or no knowledge on these parameters and thus they are difficult to optimise.

If the model outputs were still not corresponding to the measured data, then the 'not very sensitive' parameters were changed similarly to the 'very sensitive' and 'slightly sensitive' parameters as explained above. The 'not sensitive at all' parameters were not included as alterations in the model inputs would not affect the model outputs, according to the results of the sensitivity analysis (chapter 4).

The ADMS model provides specifications of some pollutants within the model interface. Bioaerosols are not specified in the model, and thus a new pollutant was created within ADMS. The pollutant properties, located within the palette of pollutant in ADMS, were kept at the model default values in the initial model run to allow the model to be set up as simply as possible.

Various modelled emission rates have been used previously when simulating the composting scenario, as detailed in Table 2-6 in Chapter 2, varying by several orders of magnitude from $2.0x10^{1}$ to $6.7x10^{10}$ (Colony Forming Units [CFU] or particles per second) for a point source (Millner *et al.,* 1980; SNIFFER, 2007). Initially an emission rate of $1x10^{5}$ CFU/m^2/s was inputted into the dispersion model to represent the approximate mid-range of the values used previously. If the modelled outputs appeared to be grossly over or under estimating the measured data, then the emission was altered when necessary, within the ranges of the emission rates used previously. It should be noted that the units used to measure bioaerosol concentrations, Colony Forming Units [CFU], are not available within the ADMS model. Therefore grams were used as a proxy unit to CFUs in the ADMS model.

5.3.3 Statistical analysis

Input parameters were modified until an adequate ‘goodness of fit’ was achieved, as described in Figure 5-1, determined by various statistical tests. The statistical tests used were based on existing modelling calibration and validation studies.

Multiple statistical tests were chosen to expose more information on the data, to enable full evaluation of the performance of the dispersion model in this specific scenario. For example, the RMSE and r and r^2 tests quantify the degree of coincidence and association respectively between the modelled and measured data (Smith *et al.*, 1996). Statistical coincidence highlights whether there is a good fit between the actual values of the modelled outputs and measured data, whereas statistical association determines whether the shape of the modelled data is similar to that of the measured data (Smith *et al.,* 1996). This is illustrated in Figure 5-4.

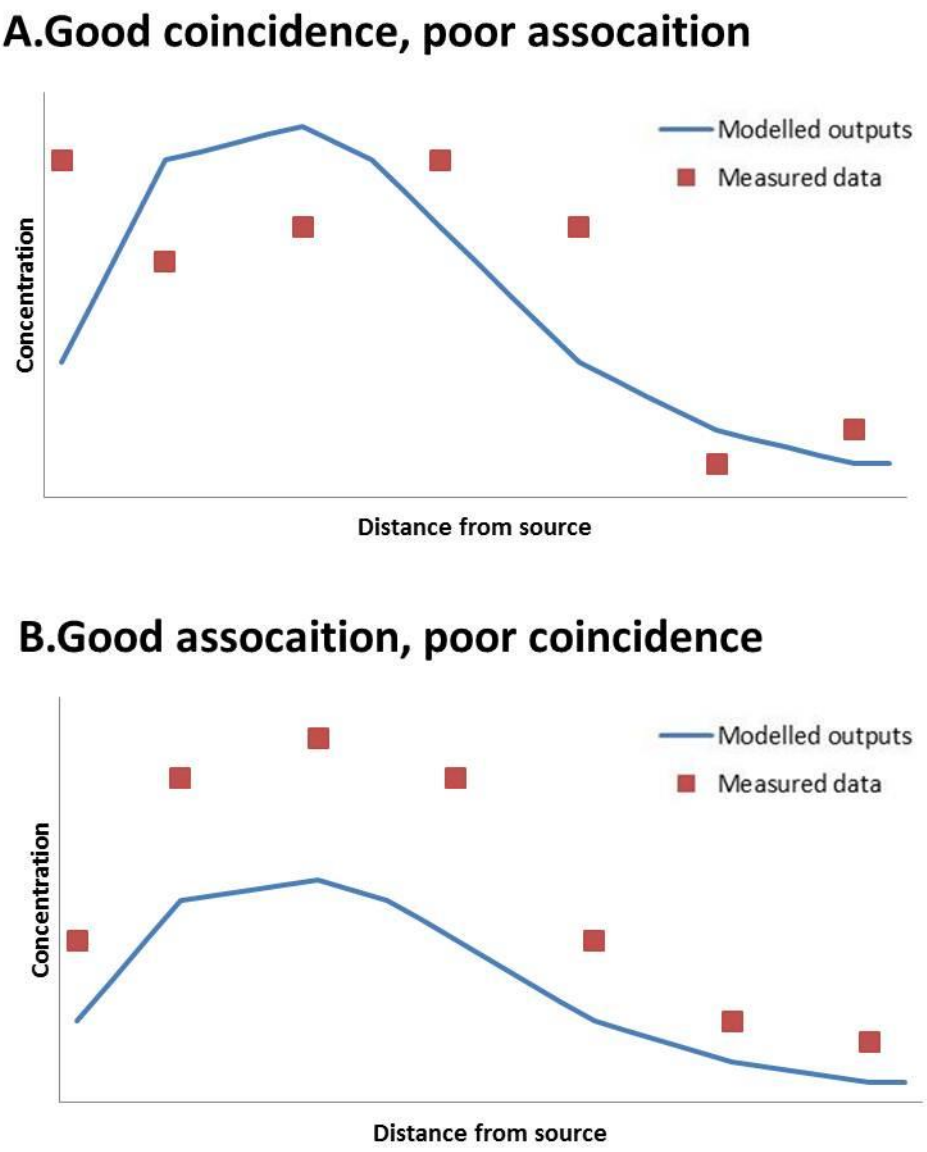

Figure 5-4 An example of the differences between statistical association and coincidence. Graph A (top), good coincidence and poor association. Graph B (bottom) Good association but poor coincidence. Based on information presented in Smith *et al.* (1996)

As a result of the potential caveats that could occur by using minimal statistical tests, as highlighted in Figure 5-4, several statistical tests were used.A summary of these tests are provided in Table 5-2, whereby:

o_i are the measured values

p_i are the modelled values

$\bar{o}$ is the mean average of the measured data

$\bar{p}$ is the mean average of the modelled data

n is the number of samples

Table 5-2 Summary of the statistical tests used throughout the model calibration

Statistic [abbreviation] (Units)	Equation	Explanation of what the statistical calculation tests	Possible ranges, with explantion
Root Mean Square Error [RMSE] (%)	$= \frac{100}{\bar{o}} \sqrt{\sum_{i=1}^{n} (p_i - o_i)^2 / n}$	RMSE provides a percentage term for the total difference between modelled and measured values, proportioned against the measured mean (Loague and Green, 1991; Smith *et al.,*1996).	The lower and upper limits of the RMSE are 0 and ∞ respectively. A value of 0 denotes a perfect fit between model outs and sampled data (Loague and Green, 1991; Smith *et al.,*1996)
Modelling Efficiency [EF]	$= \frac{(\sum_{i=1}^{n} (o_i - \bar{o})^2) - (\sum_{i=1}^{n} (p_i - o_i)^2)}{\sum_{i=1}^{n} (o_i - \bar{o})^2}$	EF assesses the accuracy of the modelled data by comparing the variance of the model outputs from the sampled values to the variance of the sampled values from the mean of the sampled data. In other words, this is a comparison of the efficiency of the ADMS model outputs to the mean of the sampled data	Values can be positive or negative with a maximum value of 1. Positive values indicate that the modelled values describe the trend of the sampled data better than simply taking the mean average of the sampled data. A negative value indicates that the mean average of the sampled data describes the sampled data better than the modelled values, and that the model is not performing sufficiently (Smith *et al.,* 1996; 1997; Loague and Green, 1991)

Statistic [abbreviation] (Units)	**Equation**	**Explanation of what the statistical calculation tests**	**Possible ranges, with explantion**
Correlation coefficient [r]	$= \frac{\sum_{i=1}^{n}(o_i - \bar{o})(p_i - \bar{p})}{(\sum_{i=1}^{n}(o_i - \bar{o})^2)^{\frac{1}{2}}(\sum_{i=1}^{n}(p_i - \bar{p})^2)^{\frac{1}{2}}}$	Measures the linear relationship between the modelled and the sampled data (Chang and Hanna, 2004). It measures the degree of association between the modelled and the sampled data, but not necessarily the coincidence, (Addiscott and Whitmore, 1987).	Values of r can lie between -1 and +1. If r equals -1 or +1 then there is perfect negative or positive correlation between the sampled and modelled data respectively. If r is equal to 0 then this indicates that there is not any correlation between the modelled and the sampled data, but this could be because the values are not linearly related, (Smith *et al.,* 1996) as non-linear relationships are not revealed by r, (Chang and Hanna, 2004).
Coefficient of determination [r^2]	$= rxr$	r^2 is a development of r, as it measures how well the modelled values can be used to predict future outcomes as well as measuring how well the modelled data fits the sampled data, (Everitt, 2006)	Values can range between 0 and 1, indicating a bad and good fit respectively between the modelled outputs and the sampled data, (Smith *et al.,* 1996)
F-Test [F]	$= \frac{(r^2/1)}{(1 - r^2)/(n - 2)}$	Measures the statistical significance of r (Smith *et al.,* 1996)	Large values of F suggest that there is a good fit between the model outputs and the sampled data, (Snedecor and Cochran, 1989)

Statistic [abbreviation] (Units)	**Equation**	**Explanation of what the statistical calculation tests**	**Possible ranges, with explantion**
Mean difference [M] (CFU/m^3)	$= \sum_{i=1}^{n} (o_i - p_i)/n$	M gives an indication of consistent errors or bias in the model, (Addiscott and Whitmore, 1987; Smith *et al.,* 1996)	M can be positive or negative; if the modelled and sampled values are the same, then M will equal 0, (Smith *et al.,* 1996)
Fractional Bias [FB]	$= \frac{(\bar{o} - \bar{p})}{0.5(\bar{o} + \bar{p})}$	FB measures systematic bias in the model, (Chang and Hanna, 2004).	Values for FB range between -2 and +2 corresponding to extreme under- or over-prediction respectively, (Radonjic and Garisto, 2012). A perfect relationship between the modeled and the sampled values would result in FB equaling 0. It should be noted that it can be possible for FB to equal 0 even if the modeled data doesn't match the sampled data due to cancelling errors, (Chang and Hanna, 2004).

In order to determine whether a suitable goodness of fit had been achieved between the modelled and sampled data, and whether model modifications should be accepted or rejected, a set of criteria were developed. The criteria were based on statistical values reported within existing successful model calibration and validation studies (CERC, 2010a; Katerji *et al.*, 2010; Hollis *et al.,* 2011; Ludwig *et al.,* 2011; and Chang *et al.,* 2012). The criteria are presented in Table 5-3.

Table 5-3 Statistical limits used in the calibration and validation, based on the statistical values presented in CERC (2010a), Katerji *et al.* (2010) Hollis *et al.* (2011), Ludwig *et al.* (2011), and Chang *et al.* (2012)

Statistic	Green category ranges	Yellow category ranges
RMSE	0 - 20	21 – 60
EF	0.75 – 1	0 – 0.74
r	0.6 – 1 -1 - -0.6	0.15 – 0.59 -0.59 – -0.15
r^2	0.6 - 1	0.4 – 0.59
M	-10 – 10	11 - 100 -100 - -11
FB	-0.5 – 0.5	0.51 – 1 -0.51 - -1

As it can be seen in Table 5-3, the statistical values reported in these studies were broad. For example, a RMSE of 10 or 60 may have been classed as a good fit in the studies and therefore resulted in what was deemed a calibrated or validated model. Therefore a colour-coded system was adopted, as shown in Table 5-3. Green was used if the statistical value was considered to give a calibrated or validated model across all studies. Yellow was used if the statistical value was considered to give a calibrated or validated model across some studies. If the value is not highlighted, then it indicates that there is a poor fit between the modelled and measured data. The F-test has not been included in Table 5-3 as it is a test of the performance of the r statistic. It does not provide any further indication of the goodness of fit between the modelled and measured data.

5.4 Results

5.4.1 Calibration stage 1

The first stage of the calibration utilised the results from the SA to help define model inputs for the calibration. As previously described, modelled outputs from the SA were compared to sampled data at 10, 100, and 250m downwind of the source, with a means with error plot. The three plots showed similar results, and thus the results are 10m downwind only are presented in Figure 5-5.

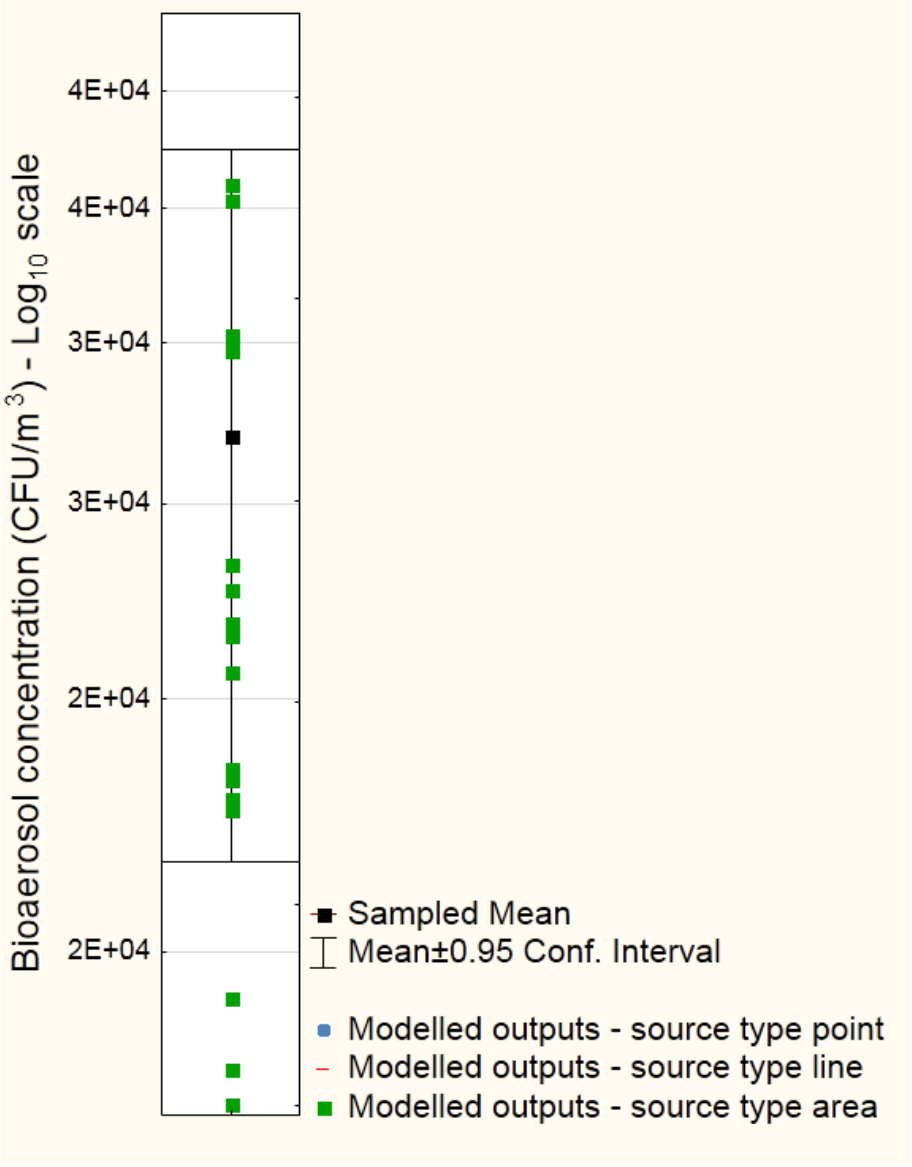

Figure 5-5 Means with error plots for comparing modelled outputs from the SA to sampled data at 10m downwind of the source. Shown with a confidence interval of 95% from the sampled mean.

Figure 5-5 shows that the majority of modelled outputs for an area source type are found within the confidence interval of the sampled data. Line source outputs were clustered below the lower confidence interval, but were in the same order of magnitude as the sampled data (data not visible). Point source outputs were found three orders of magnitude above the upper confidence interval of the sampled data (data not visible). To reiterate, similar patterns were displayed at 100 and 250 metres downwind (data not shown).

The modelled outputs which were found within the confidence interval of the sampled data in the means with error plots, at 10, 100 and 250 metres downwind of the source, were examined in more detail. This was completed by observing what model inputs were used within the dispersion model. The ranges of the inputs used within the dispersion model that achieved a good correspondence between the modelled outputs and the sampled data are reported in Table 5-4. Table 5-4 also displays what the mid-point or median of the ranges are. These mid-values were used as initial model input values for stage 2 of the model calibration.

Table 5-4 The ranges of the input values used within the dispersion model that achieved a good correspondence (within a 95% confidence interval) between the modelled outputs and the measured data. The mid-ranges of these values were used as initial model input values in calibration stage 2.

Model input parameter (units)	Range	Mid-value
Advanced model options	Not used	Not used
Source type	Area	Area
Specific heat capacity of the pollutant (J/°C/kg)	1017 - 2021	1519
Molecular mass of the pollutant (g)	19.945 – 30.703	25.324
Source height (m)	0.66 – 4.64	2.65
Pollutant exit velocity (m/s)	0.93 – 4.87	2.90
Pollutant temperature (°C)	17.4 – 52.7	35.1
Was dry deposition modelled?	No	No
Was wet deposition modelled?	No	No
Surface Roughness at the dispersion site (m)	0.42 – 1.32	0.87
Minimum value of the Monin-Obukhov length at the dispersion site (m)	128 – 189	159
Horizontal geometry of the source (m)	12.06 – 21.52	17.00
Vertical geometry of the source (m)	12.47 – 14.13	13.30
Ambient wind speed (m/s)	3.00	3.00
Sensible heat flux (W/m^2)	-10 – 0	-5
Boundary layer depth (m)	1000	1000
Ambient temperature (°C)	9.0	9.0

There is no range for some of the meteorological inputs, as shown in Table 5-4. This was due to the simplified meteorological data used within the SA model runs. As the sensitivity of the emission rate is already known, this was not included within the SA, and a value of 1 was used, irrespective of the source type. However, this is not a realistic value in the open windrow composting context. Therefore an emission rate of $1x10^5$ ($CFU/m^2/s$) was used as an initial

value in calibration stage 2, to represent the mid-range of previous emission rates used to model the composting scenario (Table 2-6).

5.4.2 Calibration stage 2

The results from calibration stage one were used to set up an initial model, as shown in Table 5-4. Parameter adjustments were made from the initial input value, within ranges applicable to the open windrow composting scenario. A good correspondence between the modelled and measured data was achieved after altering the averaging time, relating to point 4 in Figure 5-3. This was when the calibration process was halted. The buildings module was not included in the model calibration, as buildings were not present at the measured data site, as described in section 5.2. The model alterations made from the initial model inputs to achieve the calibrated model are summarised in Figure 5-6.

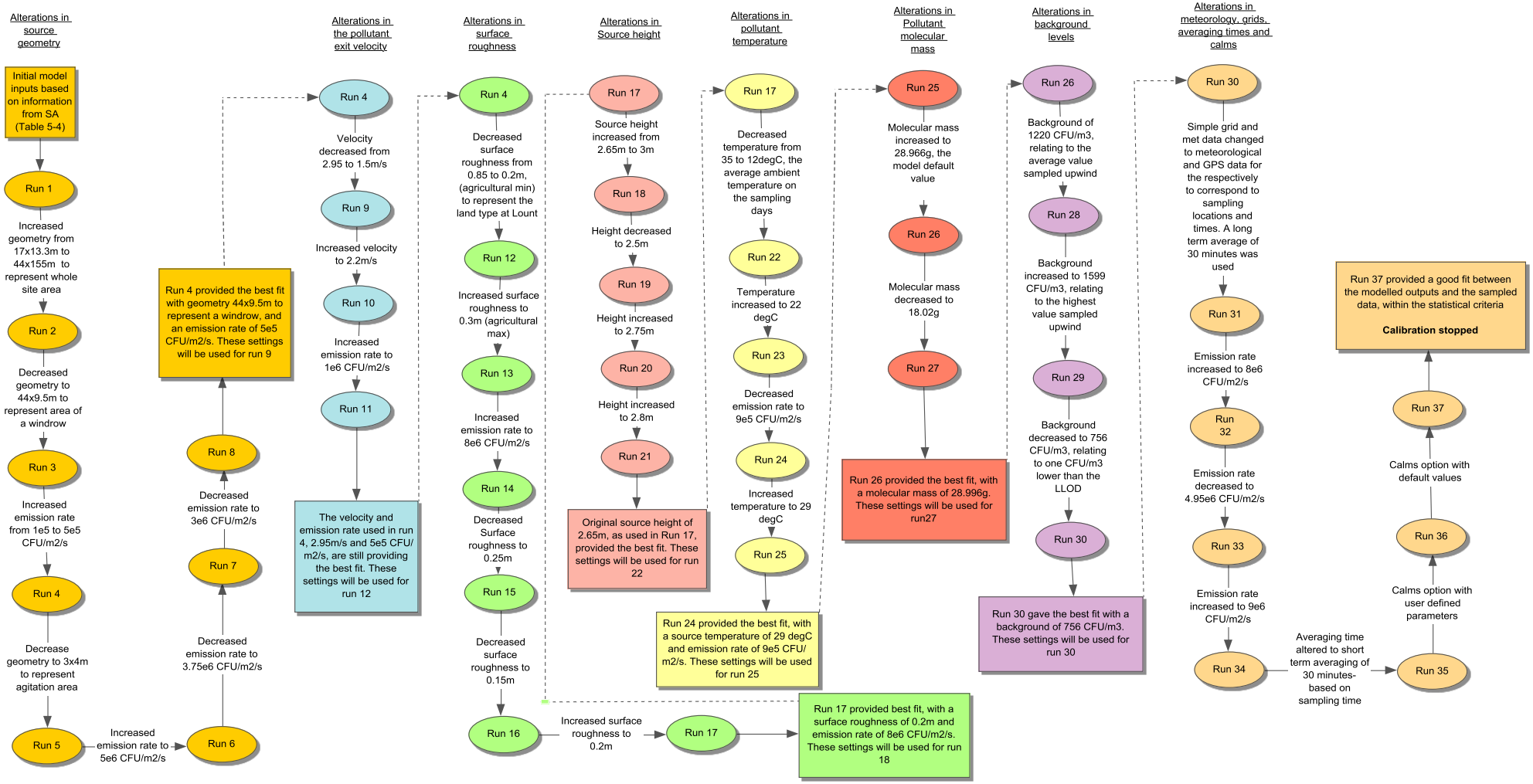

Figure 5-6 Flow diagram to illustrate the alterations made to the model during the calibration stage 2 process

The alterations completed throughout calibration stage two, as detailed in Figure 5-6, are summarised in Table 5-5.

Table 5-5 Details of the model input parameter alterations completed throughout calibration stage 2, with reference to the run numbers presented in Figure 5-6. The optimal value indicates what value provided the best fit between the modelled and the measured data.

Run numbers	Input parameter altered (units)	Values tested	Value used in the intial model run (Table 5-4)	Optimal value	Justification
1-3 and 5	Source geometry, vertical and horizontal (m)	3.0x4.0 – 44.0x 155.0	17.0 x 13.30	44.0x 9.5	Tested geometries represented the approximate area of an agitation activity (based on personal observations), the area of a windrow and the area of the whole site (based on measurements taken from aerial maps)
9-10	Pollutant exit velocity (m/s)	1.50 - 2.95	2.90	2.95	Adjusted based on preliminary measurements of the pollutant exit velocity (Chapter 7)
12-13, 15-17	Surface roughness (m)	0.15 - 0.85	0.87	0.20	Several surface roughnesses were tested, relating to the topography of the land surrounding the facility (CERC, 2010b)
18-21	Source height (m)	2.65 – 3.00	2.65	2.65	Several source heights were tested, within the ranges of the approximate height of a composting windrow (based on personal observations), and the height of screening and shredding machinery (Doppstadt, 2009; 2009b; Volvo, 2009)

Run numbers	Input parameter altered (units)	Values tested	Value used in the intial model run (Table 5-4)	Optimal value	Justification
22-23, 25	Pollutant temperature (°C)	12-29	35.1	29	Adjusted based on preliminary measurements of the pollutant temperature (Chapter 7)
26-27	Pollutant molecular mass (g)	18.02 – 28.966	25.324	28.996	Adjustments based on the results on the SA screening stages (Chapter 3)
28-30	Background option	756-1599	Not used	756	Adjustments based on concentrations of measurements taken upwind of the composting facility
31	Grid	-	Simple	Complex	Grid was altered from a simple grid, as described in section 5.3.2, to a more complex grid, based on the GPS points of the sampled data, to allow direct comparison between modelled and sampled data at each individual sampling location
31	Meterologi-cal data	-	Simple	Complex	Altered from simple meterologicaldata, based on the results of calibration stage 1 (section 5.4.1) to more complex data purchased from the UK Meterological office (Met Office, 2011a) for the sampling days and times in which sampling occurred, to allow direct comparison between the modelled and the sampled data.
31, 35	Averaging time	Short term and long term 30 minutes	Short term 30 minutes	Short term 30 minutes	Based on the sampling time used to collect the measured data, as advised by the model developers (Lad, 2012a)

Run numbers	Input parameter altered (units)	Values tested	Value used in the intial model run (Table 5-4)	Optimal value	Justification
35-37	Calms option	-	Not Used	Default value	The calms option was used as wind speeds of less than 0.75m/s were observed in the metrological file (wind speeds of less than 0.75m/s are normally not simulated within the dispersion model (CERC, 2010b))
4, 6-8, 11, 14, 24, 32-34	Emission rate ($CFU/m^2/s$)	$1x10^5$ – $9x10^6$	$1x10^5$	$9x10^6$	Various emission rates were tested, within the ranges used previously when modelling bioaerosol emissions from open windrow composting facilities, as explained in section 5.3.2

Figure 5-6 and Table 5-5 show how the model set-up has become increasingly complex throughout model calibration stage 2. This included adding meterological data taken from the weather station closest to Lount, and modelling outputs at actual sampling locations, based on GPS data, as illustrated inFigure 5-7. Table 5-5 also shows how the original pollutant exit velocity and source height input values, although adjusted, provided the best correspondance between the modelled and the measured data.

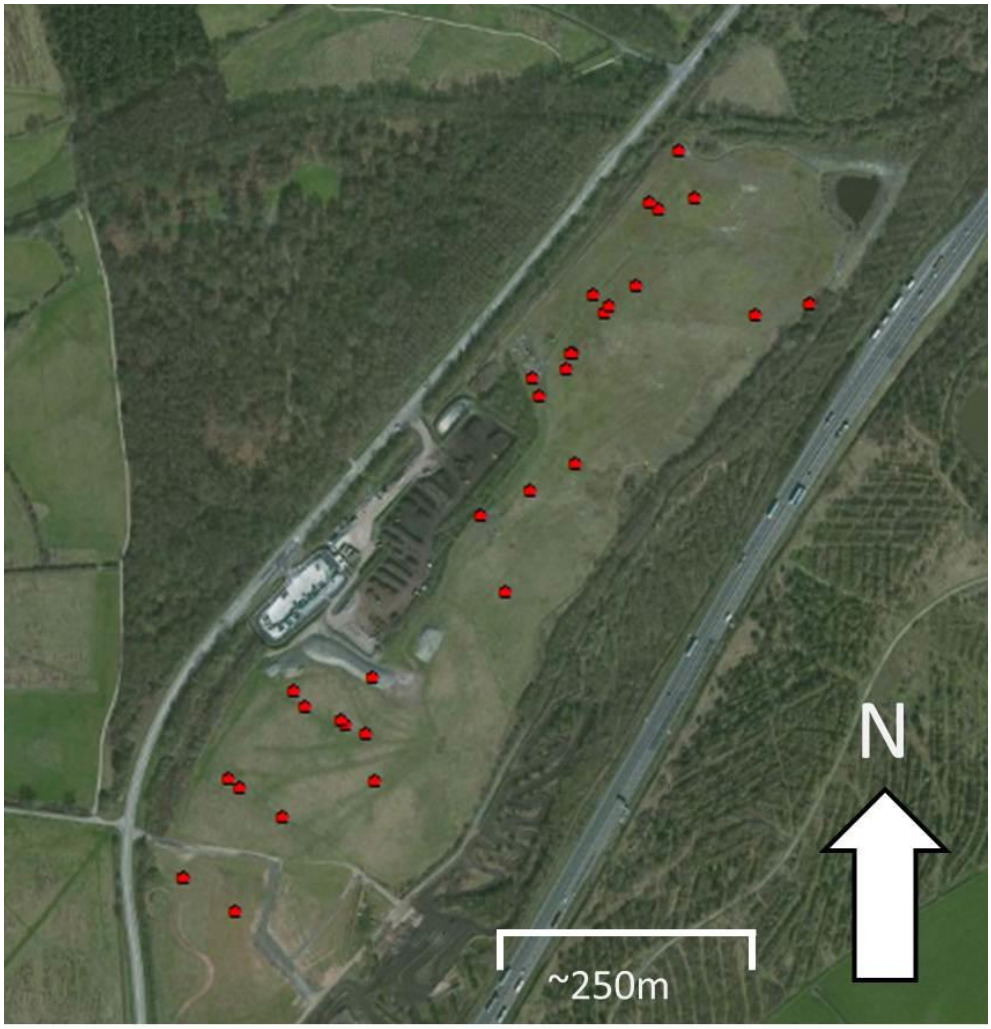

Figure 5-7 Illustration of the gridded output used in the calibrated model, based on actual GIS data collected at the measurement locations, as indicated by the red dots. Modelled output concentrations were calculated at these locations, allowing direct comparison between the modelled and measured data at the individual locations. Please note that the measurements at the locations indicated by the red dots were taken downwind of the composting facility on the day of sampling (the wind direction changed between the different sampling days) (Bing Maps 2013)

Results of the initial calibration model run and the final calibrated model run are compared in Figure 5-8, to highlight how the goodness of fit has improved by completing the model calibration. These are now referred to as the 'first' and 'final' model runs respectively. The red line in the plots denotes where the points would fall if there was a perfect fit between the modelled and the sampled data.

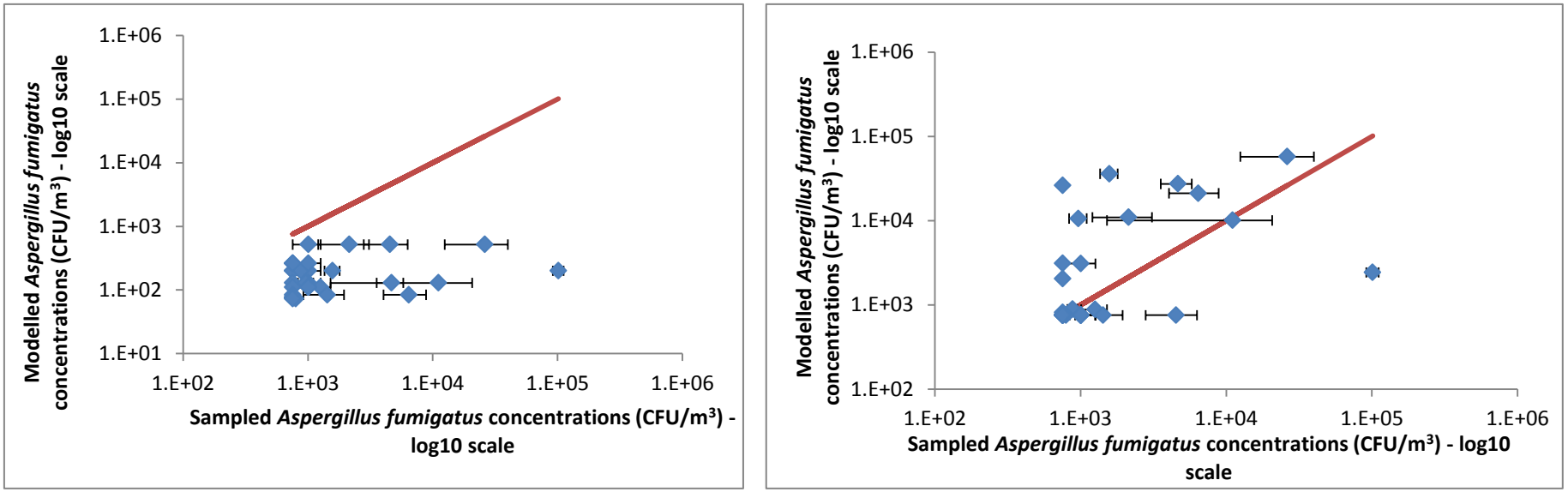

Figure 5-8 Scatter plots of all sampled data against all model outputs at downwind locations only for the first model run (run 1 - left) and the final model run (run 37 - right). The error bars denote a standard error of the mean [SEM] of the samples measured in triplicate.

Figure 5-8 shows that the first model run underestimates the sampled data as all points fall below the line of perfect fit, whereas the final model mainly overestimates the sampled data. Both plots show the variability in the sampled data, as some error bars extend over more than one order of magnitude. Figure 5-8 also shows that the points on scatter plot A, the first model run, appear to fall linearly horizontally. This has occurred due to the simplified nature in which the first model run was set up. In these plots the sampling data and the modelled outputs are compared directly. Only one modelled output was given at every distance downwind, whereas in reality two or more samples were taken at every distance downwind, as explained conceptually in Figure 5-2. This has led to one model output at a particular distance downwind being compared to several samples, hence the linear nature of scatter plot A. Sampled values do not fall below 756 CFU/m^3 on both scatter plots due to alterations of 'zero' values to one minus the LLOD, the 'worst case scenario', as described in section 5.2. In addition to this, modelled values in scatter plot B, the final model run, also do not fall below 756 CFU/m^3. This is because the background option was used in the final model run and set at this value, preventing modelled outputs of less than 756 CFU/m^3.

The statistical results for all first and final model calibration runs are compared in Table 5-6.

Table 5-6 Statistics for first and final calibration model runs. Any highlighted correspond to the limits presented in Table 5-3. All values have been rounded to 2 decimal places

Statistic	Value for the first calibration run	Value for the final calibration run
RMSE	328.80	362.61
EF	-0.09	-0.32
r	0.11	0.13
r^2	0.01	0.01
F	0.37	0.52
M	5569.11	-1497.71
FB	1.87	-0.23

Table 5-6 shows that both the first and final calibration runs have provided poor statistical values when compared to the limits presented in Table 5-3, and thus indicate that the modelled outputs do not correspond to the measured data. To reiterate, this has occurred when directly comparing the measured and the modelled data at the individual downwind locations. To examine this further, Figure 5-9 compares the modelled and the measured data at the individual downwind distances for the first and final model runs. This will allow the overall fit between the sampled and the modelled data to be observed at each distance downwind.

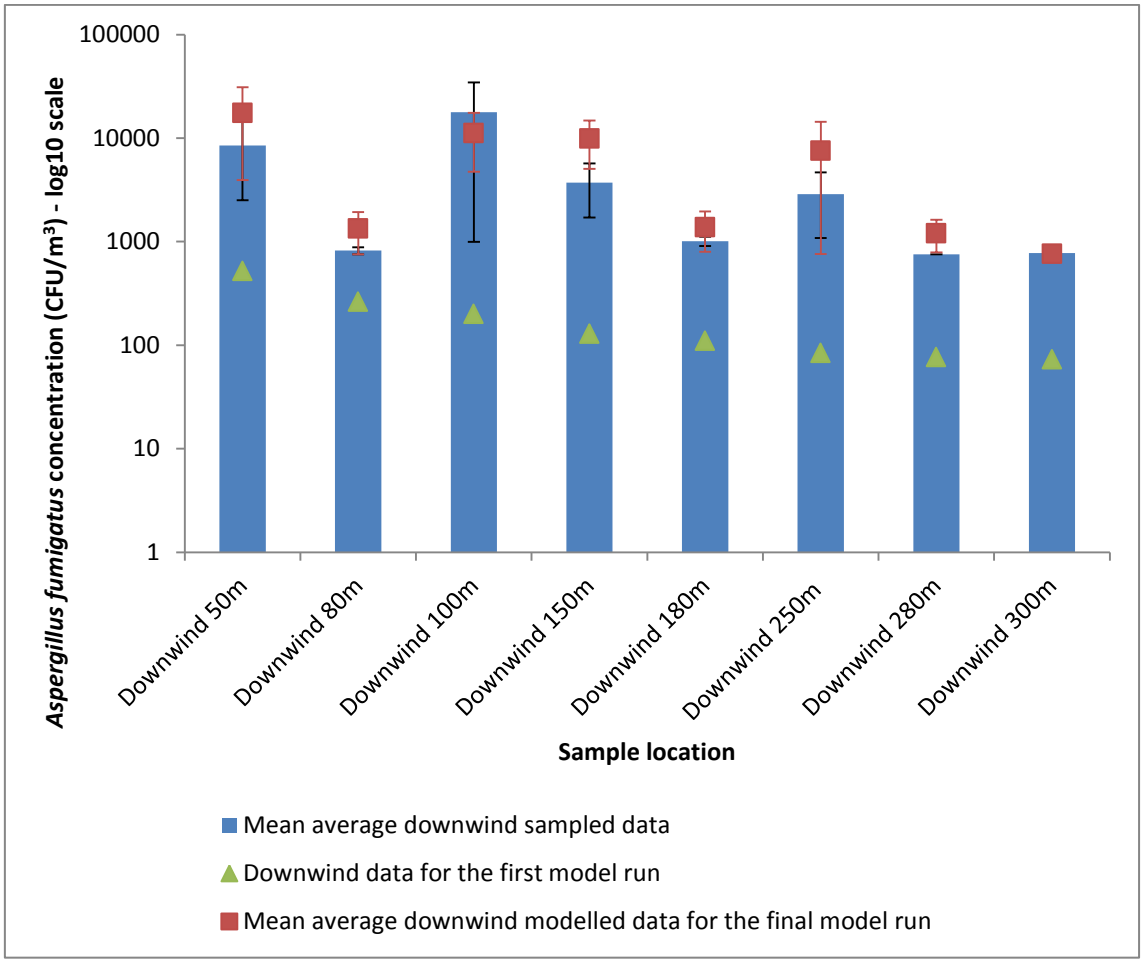

Figure 5-9 Comparison of the modelled and sampled data for the first and final model runs at each downwind location. Black error bars denote the SEM of the sampled data and red error bars denote the SEM of the final model run.

It can be seen in Figure 5-9 that the outputs for the first model run appear to follow a Gaussian dispersal profile whereas the calibrated model closely follows the shape of the sampled data, even capturing the depressions in the data at 80 and 180 metres downwind. Error bars have been displayed for the final model run only. Error bars for the first model run are not displayed as only one output was given per distance downwind, due to the simplified nature of the model set-up, as conceptualised in Figure 5-2, resulting in the SEM equalling zero. Due to the more complex nature of the model set-up in the final model run, two or more outputs were given per distance downwind to complement the sampling locations. For example, four samples were taken at 50 metres downwind on separate sampling occasions, and thus four modelled output concentrations

were calculated to correspond to the sampled data, as described in Figure 5-7. These outputs were mean-averaged, and therefore a SEM could be calculated. Visually, the mean final model run outputs represent the sampled data almost perfectly, whereas the first model run outputs grossly underestimate the sampled data by up to a factor of two. A statistical comparison is provided in Table 5-7.

Table 5-7 Statistics for the first and final model calibration runs at downwind points only. Any highlighted correspond to the limits presented in Table 5-3. '–' denotes a dividing by zero error when calculating the statistic. All values have been rounded to 2 decimal places

Model run	Downwind distance (m)	Statistic						
		RMSE	EF	r	r^2	F	M	FB
First	50	153.75	-0.59	-	-	-	7967.43	1.77
	80	69.22	-25.79	-	-	-	556.42	1.03
	100	233.07	-0.22	-	-	-	175542.07	1.96
	150	144.48	-0.81	-	-	-	3573.82	1.87
	180	90.87	-25.26	-	-	-	899.33	1.61
	250	131.19	-1.21	-	-	-	2793.69	1.89
	280	89.87	-	-	-	-	679.39	1.63
	300	90.70	-1116.05	-	-	-	704.48	1.66
Final	50	47.91	0.86	0.99	0.98	92.20	-761.73	-0.09
	80	0.02	-	-	-	-	-0.07	0.00
	100	241.99	-0.28	-0.24	0.06	0.24	10386.31	0.84
	150	339.72	-7.00	0.15	0.02	0.07	-3524.34	-0.68
	180	27.18	0.19	0.87	0.77	6.51	-93.70	-0.13
	250	57.33	0.67	0.99	0.99	20273.05	-845.34	-0.28
	280	3.81	-	-	-	-	-14.41	-0.02
	300	113.08	-1.00	1.00	1.00	-	-336.22	-0.57

Table 5-7 clearly shows that the modelled outputs for the final calibration run statistically correspond well to the sampled data, unlike the model outputs for the first calibration model run. However, it should be noted that as only one value per distance downwind was modelled for the first calibration run, as described in Figure 5-2, the mean of this data was equal to the datum itself. This caused dividing by zero errors, particularly for the r statistic, and consequently for the r^2 and F statistics also. Similarly dividing errors were experienced at 80 and 280 metres downwind for the final calibration run as the sampled values were all equal to the LLOD minus 1. The r and r^2 statistics at 300 metres downwind for the final calibration run indicate a perfect fit between the modelled and the sampled data. However, a perfect fit was not observed in the raw data (data not shown). This has occurred because only two measurements were taken at 300 metres downwind. As there were only two measured samples, which were consequently compared to two corresponding modelled outputs, the statistical calculations have resulted in seemingly perfect r and r^2 values. Any combination of values would have contributed to this result.

5.5 Discussion

5.5.1 Calibration stage 1

Results indicated that an area source is most appropriate when representing bioaerosol emissions from composting facilities. Consequently the initial calibration run was set up using an area source. The model runs that used a line or point source type were clustered slightly below or considerably above the area source data respectively, as described in section 5.4.1. This has potentially been caused by the way the different source types are treated in the dispersion model (Thomson *et al.,* 2009). Point source output concentrations are calculated centred on the coordinates of a single source. Concentrations for area and line sources are calculated by decomposing the source into a number of elements. The contribution of these elements is combined to provide a single output concentration (Thomson *et al.,* 2009). This explains why the modelled outputs of the area and line sources were clustered relatively closely together in

Figure 5-5, whereas the point sources were located several orders of magnitude from the remainder of the data. As the area source outputs corresponded to the measured data, the source was represented as an area in the initial calibration run.

5.5.2 Calibration stage 2

The order of the model input modifications were based on the results of the SA and the level of existing knowledge on the model input. Initially easy-to-modify model inputs were altered, and modifications became increasingly more complex. By completing the model modifications in this way, it is possible that the model may have been over or under calibrated. If the model was over calibrated then the model inputs will have been adjusted too specifically to the site conditions of the sampled dataset. Thus when applying the optimal model inputs to another dataset, in other words the model validation, the optimal inputs may be too specific and the modelled outputs may not correspond to the measured data. As the model input modifications became increasingly complex, and statistics were calculated between each model run, the possibility of model over calibration is unlikely. When the modelled outputs corresponded to sampled data, the calibration was halted, and the statistical thresholds used to determine this were based on values from existing studies. Therefore it is unlikely that the model was over calibrated. Under calibration is when the model inputs have not been adjusted and refined enough, and is also likely to influence the results of the model validation test. Under calibration is more likely using the methods presented in this chapter, although it is difficult to determine if this has occurred. As model inputs were adjusted until the statistical calculations equated to the values reported in Table 5-3, which were based on the statistical values calculated in successful model validation tests, it was assumed that the model had been adequately calibrated.

5.5.2.1 Comparison of the statistics calculated in this study to those reported in other model calibration and validation studies

The statistics of the final calibration model run have been compared to statistics from other model calibration and validation studies. This includes studies

performed on ADMS, and other air dispersion models in different scenarios. The comparisons are presented in Table 5-8.

Table 5-8 A comparison of the statistical analysis from several calibration and validation studies. '-' denotes that the statistic was not calculated in that particular study

Reference	Statistic						
	RMSE	**EF**	**r**	**r^2**	**F**	**M**	**FB**
This study (Table 5-7)	3.81-339.72	-7.00-0.86	-0.24-1.00	0.02-1.00	0.07-20273	-3542-10386	-0.68-0.84
CERC (2010c)	-	-	0.16 – 1.00	-	-	-	-0.44-0.80
Theobald *et al.,* (2012)	-	-	0.80 – 0.89	-	-	-	-0.78 – 0.81
Ludwig *et al.,* (2011)	16.3 – 59.4	-4.5 – 0.6	-	-	-	-	-
Hollis *et al.,* (2011)	0.02 – 0.17	0.26 – 0.94	-	-	-	-	-
Lee *et al.,* (2000)	5.95 – 129.24	-	-	0.17 – 0.99	-	-	-
Domenech *et al.,* 2012	-	-	-	0.847 – 0.997	-	-	-
Brzozowska (2013)	-	-	-	-	-	-	0.18

Table 5-8 shows that the majority of statistical results from this calibration study fell within the ranges of other studies. These statistics indicate that the ADMS model has been successfully calibrated for the composting scenario. However some of these studies claim that the model has been successfully validated even with seemingly poor statistical results. For example, the CERC (2010c) flat terrain validation study states r values as low as 0.16. From the information detailed in Table 5-2, when the value of r is approaching 0, it indicates that there is no correlation between the data (Smith *et al.,* 1996). Thus an r value of 0.16 does not indicate a good correlation between the sampled and the modelled data. Although the results from this model calibration correspond to

the results of previous model validation studies, the quality of these validation studies is questionable, when reviewing the statistical values calculated.

5.5.2.2 Comparison of the calibration model inputs to those used in previous studies

The optimal model inputs used in the final calibration model were presented in Table 5-5. These values are compared to model inputs previously used within dispersion models when simulating bioaerosol emissions from open composting facilities.

An emission rate of $9x10^6$ CFU/m^2/s was found to be the optimal value.. In comparison to previous emission rates as detailed in Table 2-6 in Chapter 2, it is apparent that this value concurs with the emission rate values previously used within dispersion models, when simulating the composting scenario. An area source was used in the calibrated model, with dimensions of 44 x 9.5 metres, which corresponds to the approximate area of a windrow. ADAS (2005), Taha *et al.* (2006; 2007), and SNIFFER (2007) have all previously modelled the composting scenario using area sources. Only the study by ADAS (2005) used an area source to model agitation activities. Dimensions of 2 x 10 metres were used by ADAS (2005), which is considerably smaller than the area used in the calibrated model. However, ADAS (2005) admitted that these dimensions were arbitrary, and did not provide a justification of why these values were used. The source height of the calibrated model was 2.65 metres. This value falls almost directly in the middle of the source heights previously used in dispersion model for this scenario, of 0 to 5 metres (Millner *et al.,* 1980; Taha *et al.,* 2006*).*Therefore the optimal fit between the modelled and measured data was achieved when modelling the source of the bioaerosol emissions as a singular relatively large area source, relating to the size of an average composting windrow at the site modelled, with a continuous emission rate. In the majority of previous modelling studies in this scenario, the emission was modelled as a point source, to represent the agitation activities (Millner *et al.,* 1980; Danneberg *et al.,* 1997; Taha and Pollard, 2004; Taha *et al.,* 2006; 2007; Drew *et al.,* 2007; SNIFFER, 2007; Tamer Vestlund, 2009). However in reality, based

on personal observations, emissions from an open windrow composting site are a complex mix of:

- Multiple small, intense sporadic high concentration releases, caused by the agitation activities carried out on site
- Large low concentration releases from un-agitated static compost

Therefore, it is likely that the area source found to be the optimal source type in this calibration study, is actually representing an average of both small, high concentration releases, and large low concentration releases.

A pollutant exit velocity of 2.95 m/s was used in the calibrated model. Consequently, this remained unchanged from the initial calibration model run, which is discussed below. Lower exit velocities have been reported in the literature; 0.19 m/s (Drew *et al.,* 2005), 0.2 m/s (Taha *et al.,* 2007) and 0.5-1.7 m/s (Tamer Vestlund, 2009). However it is not apparent how these values were measured or estimated, and thus it was assumed that these values were speculated. Similarly, a pollutant temperature of 29.1ºC was used in the calibrated model, which is positioned mid-range of the pollutant temperatures used previously in the dispersion model, 9.5 to 55°C (Taha and Pollard, 2004; Drew *et al.,* 2005; 2007; Taha *et al.,* 2006; 2007; Tamer Vestlund, 2009). However, it should be reiterated that the justified pollutant temperatures used previously within the model were based on ambient temperatures or the temperature of the compost-windrow core (Drew *et al.,* 2005; Tamer Vestlund, 2009). However the pollutant temperature is unlikely to be identical to the ambient temperature or to the core of the compost windrow, as discussed in section 2.5.3, and thus more measurements are required.

The surface roughness used in the calibration model was 0.2 metres, which is identical to the surface roughnesses reported in the literature when modelling the composting scenario (ADAS, 2005; Tamer Vestlund, 2009). However, this is not surprising as the surface roughness is representative of the type of land that the composting facility is located on or near to (CERC, 2010b). The majority of composting sites are situated in rural locations, and thus it is likely that these sites will share the same surface roughness. In addition to this, the model

allows the user to choose a surface roughness based on land type (CERC, 2010b), thus increasing the likelihood that the same surface roughness is used for the same land type.

The pollutant exit velocity and source height remained unchanged in the calibration process. Both parameters were altered, but the initial model inputs were found to provide the best fit between the modelled and the measured data. This may be due to the fact that the initial model inputs were based on the fit between modelled outputs from the SA and the measured data. This was a preliminary calibration test, and thus it is not surprising that some of the model inputs have remained unchanged, or have changed by a minimal amount.

Overall, some of the calibrated model inputs do not correspond to previous studies. In the majority of previous modelling studies, it is not apparent how the model input values used previously have been measured, estimated or justified. However, there is also limited data for some of the model input parameters, and thus there are uncertainties on what value should be used within the dispersion model. This is a probable explanation of why dispersion models have been unsuccessful at simulating bioaerosol from open windrow composting facilities.

5.5.3 Limitations

There are two main limitations of the first calibration stage. The first is related to the modelling data acquired from the SA. The second is related to the reliability of the sampled data. The limitations of the SA were discussed in Chapters 3 and 4.

As the first stage of the model calibration has utilised the data from the SA, the limitations from the SA have been transferred to this study as well. Principally it may be possible that, although justified, an incorrect model input has been used. For example, the knowledge on the specific heat capacity of bioaerosol components is limited, and thus assumptions were based on the specific heat capacities of other atmospheric gases and pollutants. However, the assumed value may still be incorrect but is based on the best available information. Nevertheless, with or without these imperfections, the results from the SA have

provided the best initial input available. Although a justified but incorrect model input may have been used in the initial model set up, it was predicted that the parameter would be altered as part of the calibration process nonetheless. As the most sensitive model input parameters were adjusted first, if the potential incorrect model remained unaltered the parameter would not be sensitive.

The second limitation of calibration stage 1, and also the major limitation of calibration stage 2 lies within the extent and accuracy of the sampled data. The sampled data used, collected by Pankhurst (2010), is the most detailed and most extensive available. To reiterate, the data was collected from 15 separate sampling visits over approximately ten months. Therefore the calibration has been performed on data that was collected in limited site and meteorological conditions. In particular, the data was consistently collected during dry weather conditions, as per the sampling protocol (AfOR, 2009). Therefore this calibration study has not included data collected during wet weather conditions, and therefore it is unknown how the model performs in the composting scenario in these conditions. However, at present, there is no data that has been collected during wet weather conditions, due to the recommendations of the sampling protocol (AfOR, 2009).

There are also potential flaws with the sampling technique adopted by Pankhurst (2010). Pankhurst (2010) reported that there are secondary peaks in the data, and that the measured data does not follow a Gaussian profile. This can be observed in Figure 5-9. Originally, the presence of these peaks was thought to be caused by buoyancy effects (Pankhurst, 2010; Pankhurst *et al.,* 2011). Buoyancy effects are caused when warm air is embedded into cooler air and rises (Oke, 1987; Beychok, 1994). This is thought to be a valid argument, particularly during turning activities, as the core of the compost can reach up to 60°C (Lacey and Crook, 1988) and is exposed to the ambient air when turned. However it is also thought that the temperature of the plume cools rapidly upon release, and thus buoyancy effects should not be observed at distances in excess of 100 metres from the release (Macdonald, 2003; Oke, 1987). It is also possible that this effect has been caused by a simple sampling error.

Bioaerosols are not visible to the naked eye, and thus when measuring their concentrations downwind of a facility, their position is estimated based on the wind direction (AfOR, 2009). However, the wind can change direction rapidly, particularly during unstable weather conditions (Oke, 1987), and this may not be detected by the sampler. Even if this is detected by the sampler, the effects cannot be mitigated as sampling is performed for at least 30 minutes in a fixed location (AfOR, 2009). Figure 5-10 illustrates the alternative theory of how the occurred in secondary peak the sampling data, caused by sampler error

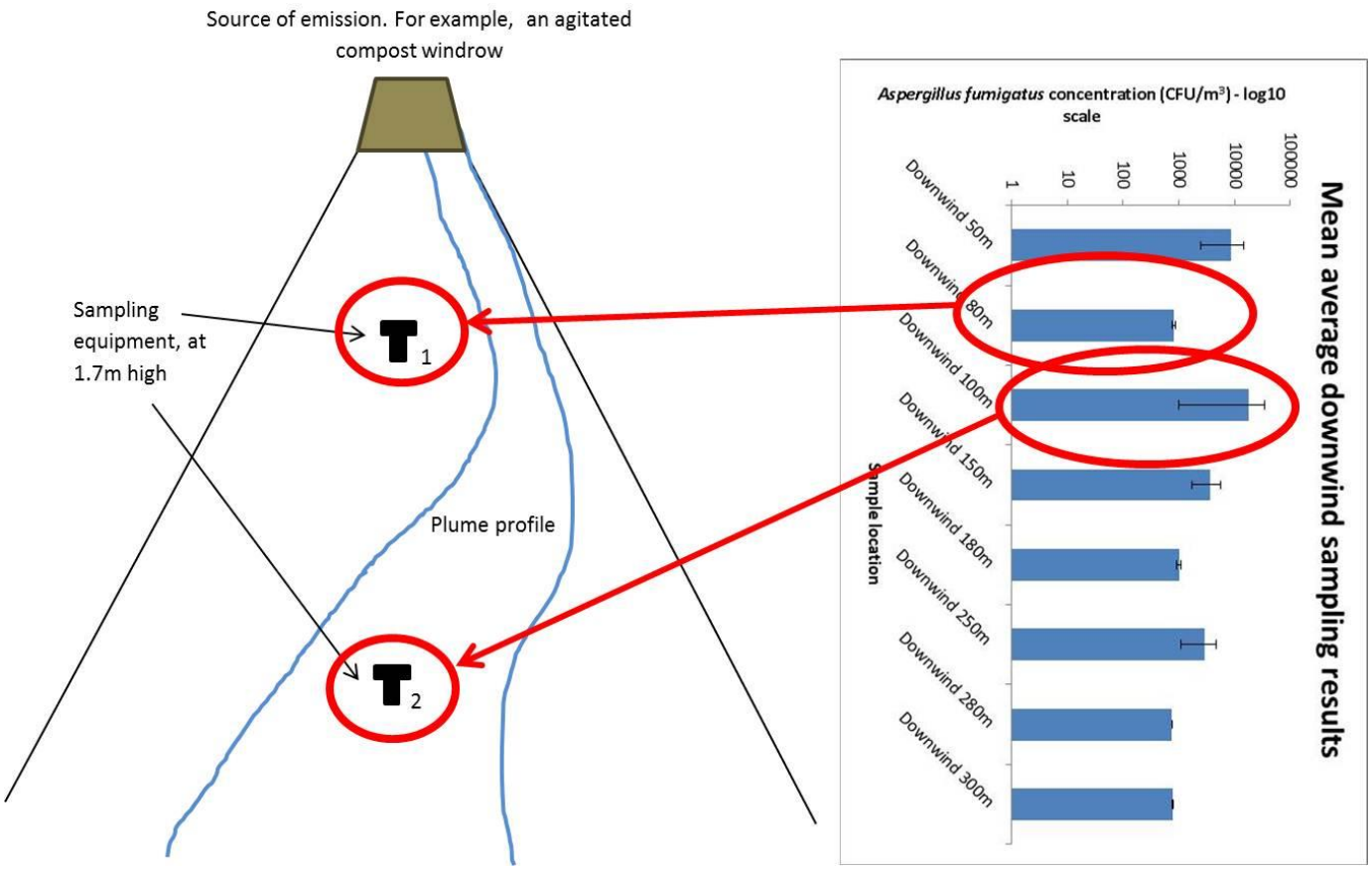

Figure 5-10 An illustration of how the alternative theory of wind direction changes may have caused the secondary peaks in the measured data, showing that sampling point T_1 is outside of the meandering plume

Therefore it is possible that the model has been calibrated to an incorrect set of measured data. The model was calibrated to correspond to the measured data, which included capturing the so called secondary peaks in the measured data. However, if these secondary peaks do not exist in reality, and have occurred due to sampler error, as described in Figure 5-10, then the model has been calibrated to a set of incorrect data. However, it should be reiterated that this was a consistent result throughout 15 different sampling events performed at Lount, and similar results were also found at a second site, Flixborough (Pankhurst, 2010). In addition to this, the sampling dataset used was the most extensive dataset available. It should also be highlighted that although the measured dataset used throughout the model calibration is the most extensive dataset available for this scenario, it is still a small dataset when compared to other calibration and validation sets in different scenarios, such as the Prairie Grass, Kincaid and Indianapolis datasets (CERC, 2010c).

There are also limitations with the sampling method itself. These limitations are described in more detail in Pankhurst (2010). In particular, the sampling method has a high LLOD, as described in section 5.2, and subsequently any apparent zero values observed in the data were altered to one minus the LLOD. Therefore the calibration has been performed on a dataset using a sampling method that is not capable of capturing bioaerosol concentrations between 1 and 756 CFU/m^3. If this information was available then the calibration may have been halted at an earlier or later stage, depending on the statistical analysis.

There are also some limitations associated with the statistics calculated in this calibration. Due to the simplified nature of the set up in the initial model run, some statistics could not be calculated when comparing the modelled and measured data at the downwind locations only. The simplified model set up only allowed one model output at each distance downwind. More than one measured value was obtained at each distance downwind. Thus when comparing these two values, the varying sampled concentrations at a singular distance downwind were compared to a constant modelled output concentration. This signified that the r statistic, and consequently r^2 and F statistics could not be

calculated. To explain this effect mathematically, the simplified model set up resulted in constant values of p_i and thus $\bar{p}$ was always equal to p_i. Therefore ($p_i - \bar{p}$) was always equal to zero, and thus resulted in a dividing error, rendering the calculations of the r, r^2 and F statistics impossible. In addition to this, some seemingly perfect r and r^2 values (=1.00) were observed at 300m downwind of the source in Table 5-7. This was due to the fact that only two samples were taken at this distance downwind, and thus were compared to two corresponding modelled outputs.

5.6 Conclusions

A model calibration, specific to the open windrow composting scenario, was performed on the ADMS model for the first time. Data from the SA was utilised and compared to the averaged sampling data to provide initial model inputs within the model in which to commence the calibration. The most sensitive parameters were adjusted first, based on the results of the SA, and were altered until the modelled outputs corresponded to the sampled data, determined by the statistical analysis. The best fit between the modelled and measured data was achieved when:

- An area source type was used

The size of the area source represented the approximate area of a composting windrow at the calibration site (Lount). Traditionally, smaller point sources have been used to represent the source of the emission (Millner *et al.,* 1980; Danneberg *et al.,* 1997; Taha *et al.,* 2006; 2007; Drew *et al.,* 2007; SNIFFER; 2007).

- A pollutant temperature of 29.0°C and pollutant exit velocity of 2.95 m/s was used

  Prior to this calibration study, modellers were not able to rationalise what pollutant temperature and exit velocity values to use within the dispersion model, resulting in a range of unjustified values.

- An emission rate of $9x10^6$ CFU/m^2/s was used

  Prior to this calibration study several emission rates covering more than

10 orders of magnitude had been used. This calibration has determined a singular emission rate, allowing the modeller to better approximate the value,

- The backgrounds option was used and set to a value of 756 CFU/m^3

This option has not been reported to have been used in previous dispersion modelling studies when simulating the composting scenario.

- Meteorological data purchased from the UK meteorological office (Met Office, 2011a) was used

This correspondedto the dates and times that sampling occurred was used, alongside the use of an additional input file to simulate the effects of low wind speeds (CALMS option)

- GPS data, collected at the sampling locations, was used to provide specified modelled outputs.
- Using a short term averaging time of 30 minutes, corresponding to the sampling time.

Although there were limitations associated with the sampling data and lack of knowledge surround the majority of modelled inputs, the model was calibrated successfully within the open windrow composting scenario, based on the statistical analysis performed.

The next chapter describes the model validation, where the optimal model inputs provided from the model calibration described in this chapter are applied to another dataset. This will determine whether this model set up is capable of simulating the bioaerosol emissions from a different composting site.

6 Model validation

6.1 Introduction

ADMS has previously been validated by the model developers, Cambridge Environmental Research Consultants [CERC] (CERC, 2012a). Validations have been completed in several conditions, including simulating emissions from sources located in areas with buildings, flat terrain, complex terrain, and combinations of these conditions. These model outputs were compared to measured data collected at the field sites detailed in the individual studies, or collected by simulating field conditions in a wind tunnel. A selection of the validation studies previously completed by CERC to assess how well the model has performed in different contexts, are summarised below and compared to the open windrow composting scenario.

The CERC validation studies completed at sites located on complex terrain have not been summarised in this section. This is because the measured data used in this chapter (described in section 6.2) was collected at a site located on falte terrain.

Flat terrain (CERC, 2010c)

This study compared model outputs to three well-known sets of measured data, Kincaid, Indianapolis and Prairie Grass. In each study, the goodness of fit between the modelled outputs of ADMS versions 4.1 and 4.2, AERMOD and ISCST3 and the sampled data were compared. The three sets of measured data are briefly described below:

- The validation on the Kincaid dataset was performed in the context of SF_6 releases from a power plant located in the USA. Pollutant releases were from a 187 metre tall stack.
- The Indianapolis dataset describe SF_6 releases from a power plant in the USA. Pollutant releases were from an 83.8 metre tall stack.
- The validation on the Prairie Grass dataset was performed in the context of SO_2 releases from natural prairie grasses 0.5 metres above ground.

At all three sites, the modelled outputs from ADMS 4.2 provided the best estimation of the sampled data. Statistical analysis showed that the correlation coefficient, r, and the Fractional Bias [FB] between the measured data and the modelled outputs ranged between 0.30 and 0.63 and -0.01 and 0.35 respectively.

Buildings – Millstone (CERC, 2010d)

Millstone is a nuclear power plant located on the Connecticut coast, USA. This validation study compared measured concentrations of SF_6 and Freon-12 to modelled outputs. These pollutants were released from stacks at heights of 29.1 and 48.3 metres high.

CERC described the ADMS modelled output data to have a “generally good agreement” with the measured data. Correlation coefficients, r, between 0.282 and 0.441 were observed, as well as FB values of -0.103 to 1.035.

Buildings – Snyder wind tunnel (CERC, 2010e)

This validation study compared modelled outputs of ADMS and ISC-Prime to measured data from experiments conducted in a wind tunnel. ISC-Prime contains the same buildings model as AERMOD. Simulated conditions within the wind tunnel were representative of steam-boiler and combustion-turbine electric-generating plants (Snyder, 1993). Air and helium were used to simulate pollutant emissions. Conditions simulated within the wind tunnel, were 1/200th of the full scale.

Pollutant concentrations were measured downwind of a building in the wind tunnel, for emissions at various stack heights (12.5-125.0 metres), stack diameters (0.1-6.68 metres), pollutant exit velocities (15-40 metres per second), and building orientations. Meteorological conditions and building dimensions remained constant throughout the experiments. Statistical analysis indicated that ADMS simulated the conditions replicated in the wind tunnel more effectively than ISC-Prime. A correlation coefficient, r, of 0.795 and FB of 0.028 was reported.

More validation studies of the buildings option are available on the CERC website (CERC, 2012a). This includes more studies where modelled outputs have been compared to measurements made on-field and to simulations within a tunnel. These studies have not been included in this section as they generally agree with the findings of the examples detailed above.

The validation studies described above were performed on non-bioaerosol pollutants, occasionally using model input parameters and ranges not applicable to the composting scenario. Therefore the conditions in which these validation studies were performed are not applicable to the open windrow composting scenario. Unlike traditional stack-like emissions, bioaerosol releases during agitation activities at open windrow composting facilities are difficult to define within a dispersion model. This is because the nature of the release is not well understood. This has been a consequence of the difficulties encountered when attempting to measure emission properties, which is difficult for two reasons:

- The pollutant release is not contained or controlled
- It is dangerous to measure at the source of emissions, due to the heavy machinery performing the agitation activities

The studies described above indicate the ADMS model is well validated and should be able to accurately simulate pollutant emissions under the conditions specified in the validation studies. However, the ADMS model has not yet been successful at predicting bioaerosol emissions from open windrow composting facilities. This has been due to a lack of model testing within this scenario, and thus there is a limited understanding of how the model works in this context. This chapter describes the first validation test on the ADMS model when applied to the open windrow composting scenario. This validation will confirm whether the optimal model inputs provided from the model calibration are applicable to other data sets or not. It will also provide a better understanding of how the ADMS model works within this context, supplying a more enhanced perception of how the model should be operated when simulating this scenario. A successfully validated model in the open windrow composting scenario would

be very advantageous, as it would be able to deliver a more continuous overview of bioaerosol emissions in space and time. Therefore, the overall objective of this chapter is 'to complete a model calibration and validation, in the context of bioaerosol emissions from open windrow composting facilities, using existing sets of measured data'.

6.2 Data overview

The data used within the model validation was collected by Pankhurst (2010), collected at the Lower Trent composting facility now referred to as Flixborough. The same sampling equipment and procedures used to collect the data that were utilised in the model calibration, were also used to collect the data at Flixborough, and are described in section 5.2 in Chapter 5. The sampling data was collected over 14 separate site visits taken between the 20th of August 2008 and the 10th of July 2009. Similarly to the calibration data collected at Lount (described in section 5.2), the data was collected using three different sampling strategies.

The location of the samples taken at Flixborough can be categorised into three categories, upwind, downwind and on-site. Again, the *Aspergillus fumigatus* data only was compared to the modelled outputs as explained in section 5.2 in Chapter 5.

Flixborough is an open windrow composting facility located north of Scunthorpe. The site processes waste collected from the kerbside and from civic amenity sites in a ratio of approximately 2:1 respectively (Pankhurst, 2010). The site is relatively flat, and is located on an impermeable concrete pad. Flixborough is situated on the southern edge of an industrial estate, meaning that the nearest sensitive receptors are less than 100 metres away. This is unusual as sites are normally located in rural areas, and as a result,at least 250 metres away from sensitive receptors. As the site is located near an industrial estate, there is also an abundance of buildings located to the north of the site. The River Trent borders the western edge of the site, providing complex local meteorology. These features are illustrated in Figure 6-1.

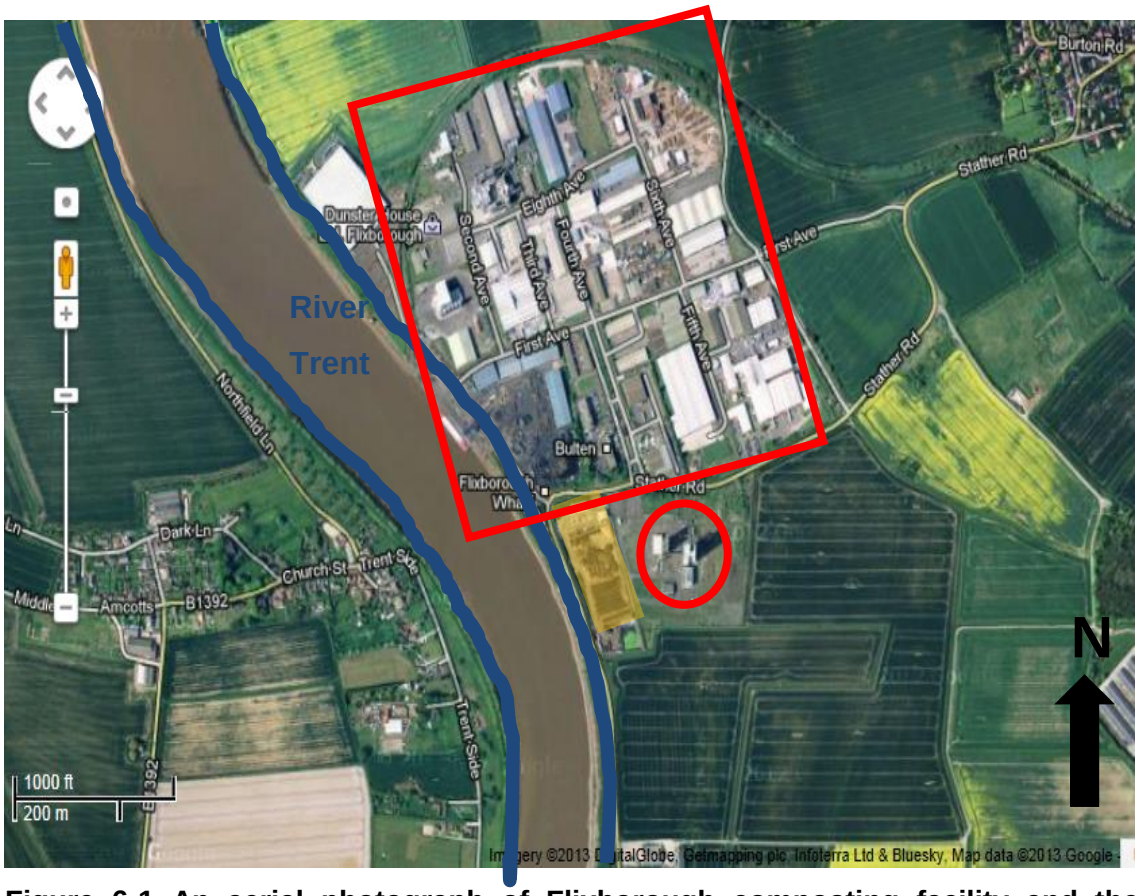

Figure 6-1 An aerial photograph of Flixborough composting facility and the surrounding area. The location of the site is highlighted in orange, and the proximity of complex features are highlighted in blue(The River Trent) and red (building belonging to the industrial estate). (Google Inc ©, 2013)

Overall, as depicted in Figure 6-1, this is a complex site and provides many challenges to a modeller. Despite these complexities, the data collected from this site, along with the data used in the model calibration, is the most extensive sampling dataset available, hence why it is used in this validation study. Moreover it will test the ability of the dispersion model to simulate emissions from complex sites, within the limits of current knowledge and data.

6.3 Approach

The optimal model inputs gained from the model calibration were used to set-up the ADMS model for the validation study, as shown in Table 5-5. As the measured data used for the validation has been collected from a different site

than the measured data that was used throughout the calibration, some alterations were made to the optimal inputs to reflect the disparities between the two measurement sites. These alterations are described and explained in Table 6-1. The model outputs were compared to the measured data collected at Flixborough, using the same statistical methods as described in section 5.3.3 in Chapter 5. Similarly to the calibration stage, the modelled outputs were compared to measured *Aspergillus fumigatus* data collected at Flixborough only.

Table 6-1 A comparison of the optimal model inputs provided by the model calibration with the model inputs used in the model validation. 'N/A' denotes 'not applicable'.

Model input parameter (units)	Optimal value achieved in the model calibration as detailed in Table 5-5	Input value used in the model validation	Justification if there is a difference between the values used in the model calibration and validation
Advanced options used?	None used	None used	N/A
Additional model input files used?	Yes - Calms option, to allow wind speeds below 0.75m/s to be modelled	Yes - Calms option, to allow wind speeds below 0.75m/s to be modelled	N/A
Source type	Area	Area	N/A
Source geometry (m)	44.0 by9.5	56.4 by8.4	During the model calibration, several area source geometries were tested, as detailed in Figure 5-6 and Table 5-5 in Chapter 5. Results from the model calibration suggested that an area source with dimensions representing the length and width of a composting windrow provided the best fit between the modelled outputs and the measured data. Therefore the length and width of a windrow from the validation sampling site was used. This was estimated using aerial maps in geospatial software, ArcMap™ (ArcGIS®, 2012)
Source height (m)	2.65	2.65	-
Pollutant specific heat capacity (J/°C/kg)	1519	1519	N/A

Model input parameter (units)	**Optimal value achieved in the model calibration as detailed in Table 5-5**	**Input value used in the model validation**	**Justification if there is a difference between the values used in the model calibration and validation**
Pollutant molecular mass (g)	28.996	28.996	N/A
Pollutant exit velocity (m/s)	2.95	2.95	N/A
Pollutant temperature (°C)	29.0	21.6	Preliminary pollutant temperature measurements indicated that the pollutant temperature was consistently higher than the ambient temperature, as detailed in Chapter 7. The optimal pollutant temperature used to achieve a calibrated model was 29 0ºC. This was 2.9ºC higher than the highest ambient temperature in the observed meteorological input file used in the calibrated model. As a different meteorological input file was used for the model validation, the pollutant temperature was altered to be 2.9ºC higher than the highest ambient temperature observed in this meteorological file.
Emission rate ($CFU/m^2/s$)	$9x10^6$	$9x10^6$	N/A
Surface roughness (m)	0.2	0.2	N/A

Model input parameter (units)	Optimal value achieved in the model calibration as detailed in Table 5-5	Input value used in the model validation	Justification if there is a difference between the values used in the model calibration and validation
Meteorological data	Purchased from the UK Meteorological Office (Met Office, 2011a) collected at Sutton Bonington, which is the closest weather station to Lount. Sutton Bonington is located approximately 15km north east of Lount.	Purchased from the UK Meteorological Office (Met Office, 2011a) collected at Leconfield, which the closest weather station to Flixborough. Leconfield is located approximately 32km north east of Flixborough.	Site specific meteorological data
Background option used?	Yes, with a value of 756 CFU/m^3	Yes, with a value of 756 CFU/m^3	N/A
Grid	Cartesian coordinate system used, with outputs calculated at specified points based on GPS data taken at the sampled locations. Outputs calculated at 1.7m, corresponding to the height of the sampling equipment (Pankhurst, 2010)	Cartesian coordinate system used, with outputs calculated at specified points based on GPS data taken at the sampled locations. Outputs calculated at 1.7m, corresponding to the height of the sampling equipment (Pankhurst, 2010)	Site specific GPS data, corresponding to the locations where bioaerosols were sampled
Averaging time (minutes)	Short term 30	Short term 30	N/A

6.4 Results

The results were analysed similarly to the data in the model calibration. All sampling results, collected at downwind locations only, are compared to the corresponding modelled outputs by means of a scatter plot in Figure 6-2.

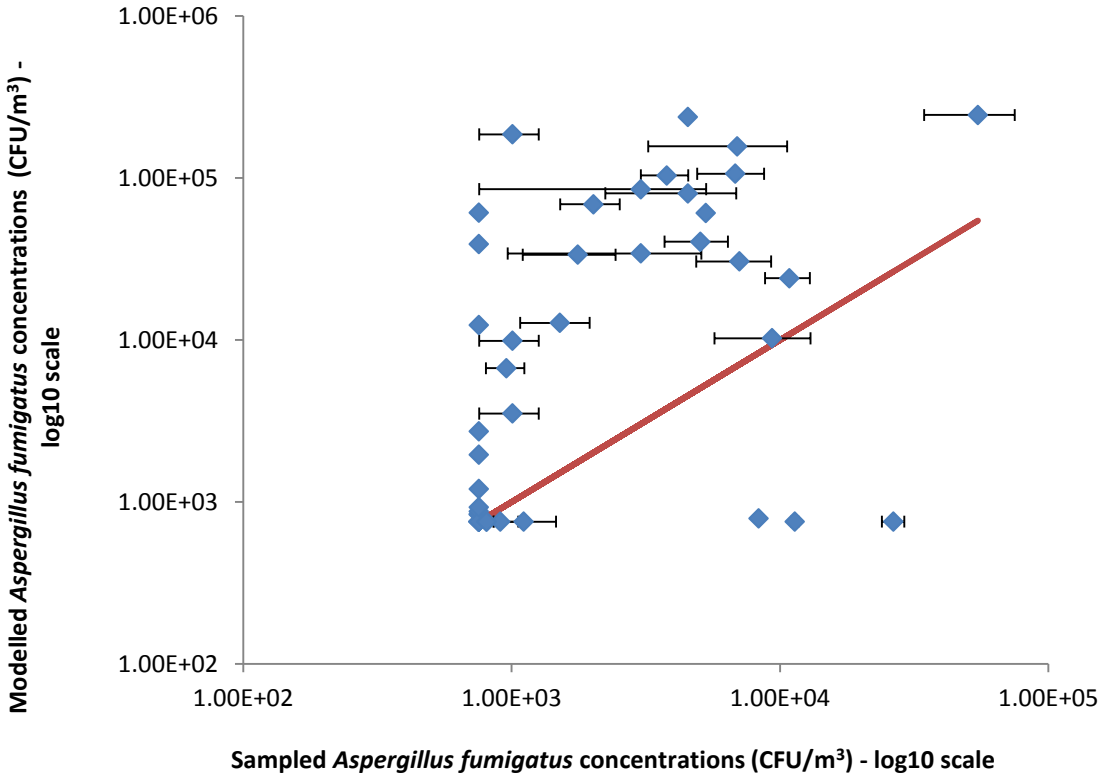

Figure 6-2 Scatter plot of all sampled data, collected at downwind locations only, plotted against all corresponding modelled outputs for the validation. The error bars denote the Standard Error of the Mean [SEM] of the triplicated samples. The red line signifies where the points would fall if the modelled outputs corresponded perfectly to the measured values.

Figure 6-2 indicates that the model is mainly over-estimating the sampled values, as the majority of points fall above the red line of perfect fit. Similarly to Figure 5-8 in Chapter 5, the sampled values do not fall below 756 CFU/m^3. This is due to all sampled values which appeared to be equal to zero were altered to one lower than the Lower Limit of Detection [LLOD]. Likewise, the modelled values do not fall below 756 CFU/m^3, because the background option within the

dispersion model was used, also corresponding to one less than the LLOD. The statistical analysis of this data, calculated as described in section 5.3.3 is presented in Table 6-2.

Table 6-2 Statistics from the comparison of all the sampled data to the corresponding modelled outputs for the model validation. Any highlighted values correspond to the limits presented in Table 5-3. All values presented are rounded to 2 decimal places.

Statistic	Value
Root Mean Square Error [RMSE]	914.58
Modelling Efficiency [EF]	-9.74
Correlation Coefficient [r]	0.31
Coefficient of determination [r^2]	0.09
F-test [F]	7.75
Mean Difference [M]	-33207.27
Fractional Bias [FB]	-1.21

It can be observed in Table 6-2, based on the statistical analysis, the modelled outputs do not correspond well to the sampled data. Similarly to the model calibration, the data was analysed again, to compare the modelled and sampled data at each sampled distance downwind. This is illustrated graphically in Figure 6-3.

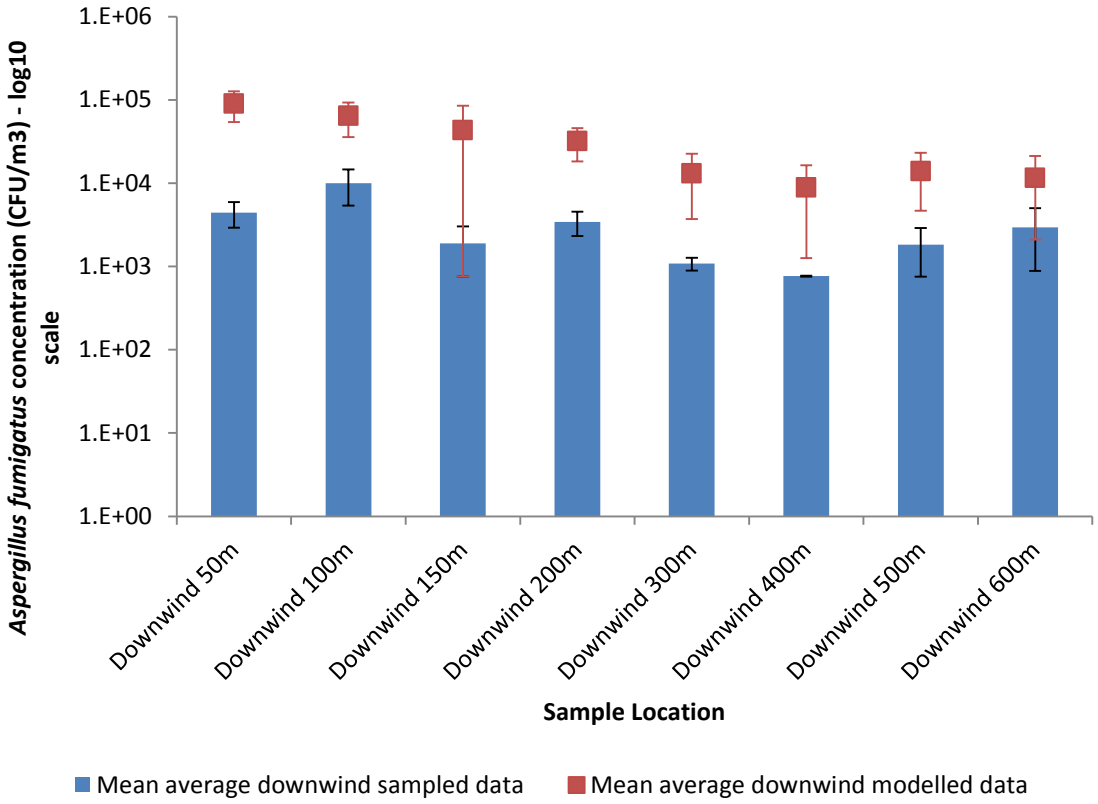

Figure 6-3 Validation results for each downwind location. Black error bars denote the SEM of the sampled data, and the red error bars the SEM of the modelled data.

Figure 6-3 shows that the model does appear to consistently overestimate the sampled data, approximately by one order of magnitude. Statistical analysis of the data at locations downwind of the site only is presented in Table 6-3.

Table 6-3 Downwind location specific statistics for the validation model run. Any highlighted cells correspond to the limits presented in Table 5-3. '-' denotes a diving by 0 error when calculating the statistic. All values presented are rounded to 2 decimal places.

Distance downwind (m)	Statistic						
	RMSE	EF	r	r^2	F	M	FB
50	1003.99	-440.62	-0.33	0.11	0.12	-30831.40	-1.55
100	835.22	-28.68	0.48	0.23	3.06	-564844.21	-1.41
150	2809.33	-2187.26	1.00	1.00	-	75193.85	-1.82
200	879.09	-79.91	0.32	0.10	0.92	-11950.71	-1.27
300	2110.40	-2465.42	0.73	0.54	10.44	-10857.52	-1.67
400	1722.52	-	-	-	0.21	-5968.28	-1.59
500	866.44	-71.67	0.99	0.99	654.09	-8710.22	-1.41
600	405.82	-15.77	0.99	0.99	4362.51	-7023.46	-1.09

The statistical analysis presented in Table 6-3 indicates that the modelled outputs do not correspond well to the sampled data, indicating that the model is not performing well on this particular dataset. However, good r and r^2 values were detected, indicating that the modelled outputs are correlated to the sampled data, confirming that the modelled outputs follow the overall trend of the sampled data.

6.5 Discussion

Based on the statistical analysis presented in Table 6-2 and Table 6-3, the modelled outputs are not corresponding well to the sampled data and thus the model is not performing well when applied to the Flixborough site. However, as explained in sections 5.2 and 6.2, the sites where the measured data were collected are very different. During the model calibration, one of the adjustments that should have been made was associated with the presence of buildings, as detailed in Figure 5-3. However there were no buildings present up or downwind of the site, and thus this option was not considered. Therefore the optimal model inputs provided by the model calibration did not include the buildings modelling option in ADMS. The site used for the model validation does contain

a substantial amount of buildings downwind of the composting facility. As the buildings option was not considered in the model validation, this potentially explains why the model outputs have not corresponded to the sampled data. Additionally, many of the optimal model input values discovered by completing the model calibration were altered in the model validation stage. This was intended to reflect the differences between the sites at which the measured data was collected from. Therefore it is possible that this has in fact worsened the performance of the model. Therefore the optimal model inputs discovered by completing the calibration stage should be tested and compared to the results presented in this chapter to establish whether it has worsened the fit between the modelled and measured data or not.

These theories are tested in Chapter 7.

6.6 Conclusions

This chapter has presented the first model validation study, specific to the open windrow composting scenario, performed using ADMS. The optimum model inputs from the model calibration were inputted into the dispersion model with some modifications to reflect disparities between the calibration and validation data collection sites. Statistical analysis of the data showed that the modelled outputs were not corresponding to the measured data, indicating that the model was performing poorly. However, as the presence of buildings was not considered in the dispersion model, and some adjustments from the optimal model inputs were made, it is possible that these factors account for the apparent substandard correspondence between the modelled and measured data. The next chapter describes additional model validation tests to examine whether these adjustments will improve the fit between the modelled and measured data.

7 Additional model validation tests

7.1 Introduction

A model validation was completed using ADMS in the open windrow composting context for the first time in Chapter 6. However, results indicated that the model was not performing adequately when compared to measured data. It was hypothesised that this may have been caused because:

- The model calibration was completed without the use of the buildings module. The measured data used throughout the model calibration was collected at a site where no buildings were present, and therefore it was not necessary to include the buildings module. However, the site at which the measured data for the model validation was collected was located in an area where multiple buildings were located around the site. Therefore the lack of use of the buildings module may have caused the model to perform inadequately
- Site-specific modifications were made to selected optimal model inputs to reflect the differences between the two data collection sites. These alterations may have worsened the fit between the modelled and measured data

These hypotheses are tested in this chapter, in sections 7.2, 'buildings test' and 7.3 'site-specific modifications test' respectively.

7.2 Buildings test

7.2.1 Approach

The model inputs as described in Table 6-1 were inputted into the dispersion model with the addition of the buildings options. All buildings situated near to the sampling locations were included. The building dimensions and orientations were estimated using aerial photographs on geographical software packages such as ArcMap™ (ArcGIS®, 2012) and Google™ Earth (©Google, 2012). ADMS is only capable of modelling point sources when using the buildings option, and will only simulate the turbulent effects around convex buildings.

Therefore the area source, which was discovered to be the optimal source type in the model calibration, was converted into a series of 14 point sources, each with a diameter of 4 metres. These point sources represented the extent of the original area source. The emission rate for an area source has units of CFU/m^2/s, whereas the emission rate for a point source has units of CFU/s. Therefore the optimal emission rate of $9x10^6$ CFU/m^2/s, discovered during the model calibration, was also converted to correspond to the 14 point sources. After consultation with the ADMS model developers (Lad, 2012b), this conversion was completed by multiplying the original emission rate, $9x10^6$ CFU/m^2/s by the dimensions of the area source (56.4 by 8.4 metres), and then dividing by 14, to provide an emission rate for each individual point source. This resulted in an emission rate of $3.05x10^8$ CFU/s for each individual point source. Additionally all non-convex buildings were enlarged to a rectangular shape.

7.2.2 Results

A scatter plot of all the sampled data, collected at downwind locations only, is compared to the corresponding modelled outputs and presented in Figure 7-1.

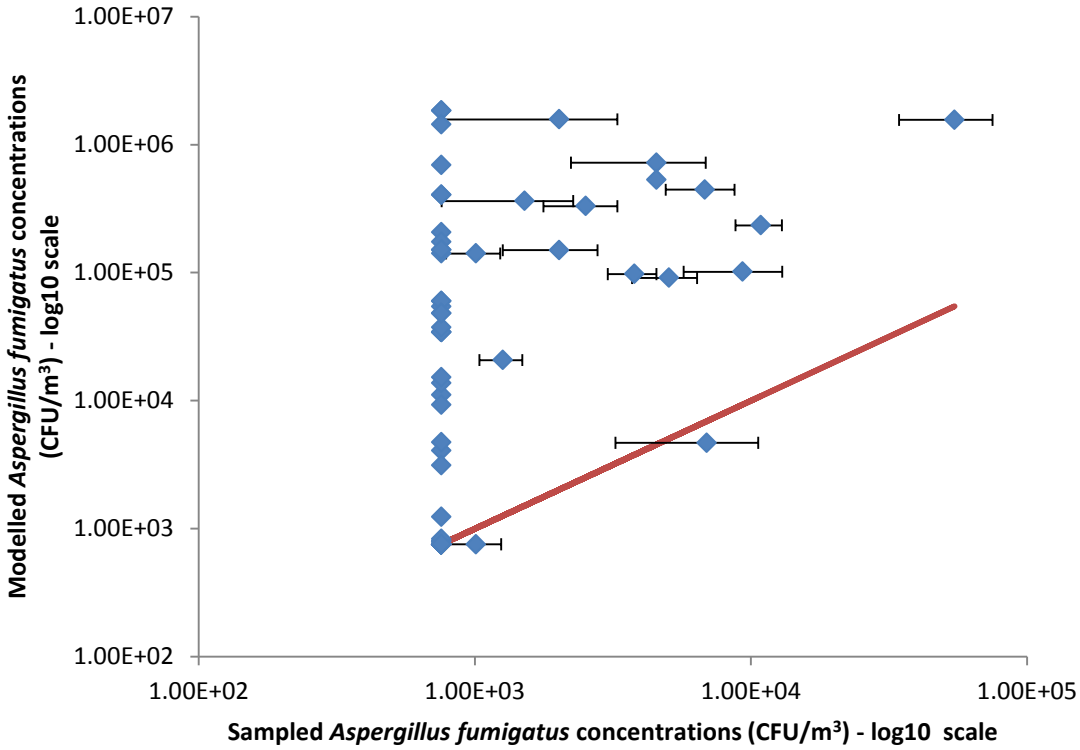

Figure 7-1 Scatter plot of the sampled data collected at downwind locations only, plotted against the corresponding modelled outputs for the model validation, when the buildings option was used. The error bars denote the SEM of the triplicated samples. The red line signifies where the points would fall if the modelled outputs corresponded perfectly to the measured values.

Figure 7-1 shows that the model is mostly overestimating the measured data. The statistical analysis of these results are presented in Table 7-1, alongside the statistical values for the validation run without the use of buildings options, originally presented in Table 6-2.

Table 7-1 Statistics from the comparison of all the sampled data, collected at downwind locations only, to the corresponding modelled outputs for the model validations 1) with the use of the buildings options and 2) without (as presented in Table 6-2). Any highlighted values correspond to the limits presented in Table 5-3. All values presented are rounded to 2 decimal places.

Statistic	1) with buildings	2) without buildings, as originally presented in Table 6-2
RMSE	21079.46	914.58
EF	-5172.30	-9.74
r	0.39	0.31
r^2	0.15	0.09
F	12.20	7.75
M	-196327.03	-33207.27
FB	-1.96	-1.21

The statistical analysis in Table 7-1, suggest that the modelled outputs do not correspond to the measured data when using the buildings options. Moreover, the statistics for the validation run that used the buildings option show that the correspondence between the modelled and sampled data is worse than the original validation run where the buildings options were not used.

When analysing the results from the original validation run where the buildings options were not used, the measured and modelled data were compared at each individual downwind distances. For the purposes of fully evaluating the 'buildings test' and comparing the results to the original model validation, the modelled and sampled data were compared at each individual downwind distance. Results from this analysis are depicted in Figure 7-2.

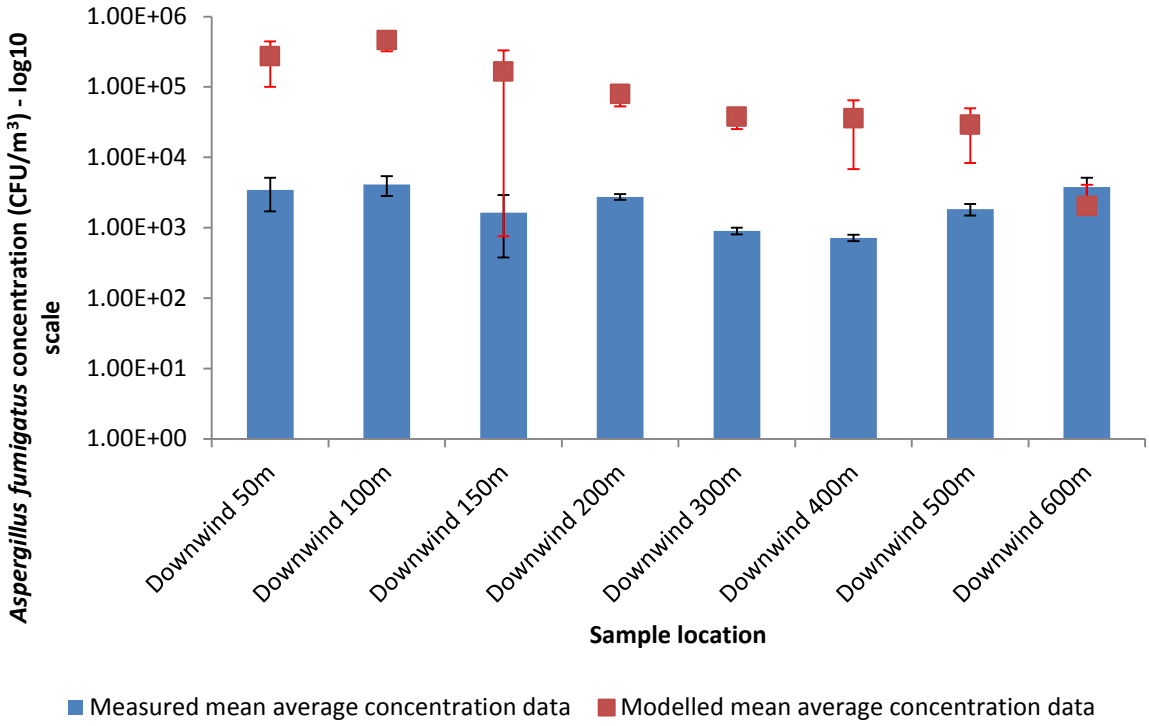

Figure 7-2 Model validation results for each downwind location, when using the building option. Black error bars denote the SEM of the sampled data, and the red error bars the SEM of the modelled data.

The graphical results presented in Figure 7-2 indicate that, with the exception of the results at a distance of 600 metres downwind, the model is mostly overestimating the measured data by at least one order of magnitude. It is also observed that generally the modelled outputs follow the trend of the measured data. This is confirmed in the statistical analysis presented in Table 7-2.

Table 7-2 Downwind location-specific statistics for the validation model run, for 1) when the buildings option was included and 2) without, as originally presented in Table 6-3. Any highlighted cells correspond to the limits presented in Table 5-3. '-' denotes a diving by 0 error when calculating the statistic.

Distance downwind (m)	Statistic													
	RMSE		EF		r		r^2		F		M		FB	
	1)	2)	1)	2)	1)	2)	1)	2)	1)	2)	1)	2)	1)	2)
50	11685	1004	-26548	-441	0.04	-0.33	0.00	0.11	0.00	0.12	-268990	-30831	-1.95	-1.55
100	19392	835	-5180	-29	0.33	0.48	0.10	0.23	2.52	3.06	-457792	-564844	-1.96	-1.41
150	14134	2809	-68715	-2187	1.00	1.00	1.00	1.00	-	-	-163975	75194	-1.96	-1.82
200	4833	879	-3859	-80	0.76	0.32	0.58	0.10	22.10	0.92	-78008	-11951	-1.94	-1.27
300	6112	2110	-22968	-2465	0.00	0.73	0.00	0.54	0.00	10.44	-36847	-10858	-1.91	-1.67
400	10967	1723	-808965	-	0.20	-	0.04	-	0.21	0.21	-34987	-5968	-1.92	-1.59
500	2391	866	-554	-72	0.99	0.99	0.98	0.99	108.96	654.09	-27298	-8710	-1.76	-1.41
600	149	406	-2	-16	-1.00	0.99	1.00	0.99	-	4362.51	1758	-7023	0.60	-1.09

The statistical analysis in Table 7-2 indicates that the model is not performing well when compared to this particular dataset. However the r and r^2 values show that the modelled outputs are well correlated to the sampled data, confirming that generally, the modelled outputs follow the overall trend of the sampled data. Furthermore, the statistical values presented in Table 7-2 indicate that the correspondence between the modelled and sampled data is worse when the buildings module was used than when the buildings module was not used.

7.3 Site specific modifications test

7.3.1 Approach

The model inputs that were adjusted prior to the model validation test, as detailed in Table 6-1, were altered to the original input values discovered to be optimal during the model calibration stages.. The source geometry, pollutant temperature and meteorological data were altered one-at-a-time [OAT] to observe whether changing that input parameter resulted in an improved or exacerbated fit between the modelled and measured data. To clarify, the tests completed were:

1. Pollutant temperature was altered from 21.6ºC to 29ºC (and then returned to 21.6ºC, when other parameters were altered)
2. Source geometry was changed from 56.4 by8.4 metres to 44.0 by9.5 metres (and then returned to 56.4 by8.4 metres, when other parameters were altered)
3. Meteorological data was changed from data collected at the weather station closest to Flixborough to data collected at the weather station closest to Lount. Weather conditions at the times and dates when sampling occurred at Flixborough were selected from the Lount meteorological data. It is appreciated that altering the meteorological data in this way is an abstract approach. However this alteration was completed nonetheless to determine whether this input was causing, or partially causing, the poor fit between the modelled and measured data

observed in section 6.4. It should be noted that use of the calms option remained unchanged, as the altered meteorological file included wind speeds of less than 0.75 metres per second. Without the use of the calms option, this data would not be modelled.

In keeping with the results analysis already presented in this chapter, and Chapter 6, the modelled and measured results were analysed in two ways. Firstly, each individual measured data was compared to the corresponding modelled outputs, at all locations downwind of the composting facility. Secondly, the modelled and measured data was compared at each measurement distance downwind.

7.3.2 Results

Graphically the comparisons between the individual modelled and measured data at sampled locations downwind of the site are similar to those presented in section 6.4 and thus are not presented. Table 7-3 compares the statistical analyses of the additional model validation tests to the initial validation, originally presented in Table 6-2. A comparison between this data and the validation model run that utilised the buildings options has not been made, as the use of that option worsened the fit between the modelled and sampled data.

Table 7-3 Statistics from the comparison of the sampled data to the corresponding modelled outputs at downwind location only for a) the original model validation, 1) altered pollutant temperature, 2) altered source geometry and 3) altered meteorological data. Any highlighted values correspond to the limits presented in Table 5-3. All values presented are rounded to 2 decimal places.

Statistic	a) Initial model validation value, originally presented in Table 6-2	Additional model validation tests		
		1) Pollutant temperature	2) Source geometry	3) Meteorological data
RMSE	1520.66	968.47	1218.48	1124.30
EF	-54.97	-6.62	-11.07	-9.27
r	0.48	0.44	0.37	0.42
r2	0.23	0.19	0.14	0.18
F	13.33	24.57	16.59	23.10
M	-33028.70	-23098.66	-29550.23	-26158.67
FB	-1.58	-1.23	-1.34	-1.28

Statistically, when considering all of the sampling locations as illustrated in Table 7-3, all model alterations provide an improved correlation between the sampled and the modelled data when compared to the initial validation, as indicated by the r and r^2 values. Additionally, M values have all improved when compared to the original validation. However RMSE values have consistently worsened, as have FB values. EF values improved when altering the pollutant temperature and meteorological data, but worsened when altering the source geometry. These statistics are inconclusive to determine whether any of the additional validation tests have improved or worsened the fit between the modelled and sampled data. The downwind data was analysed in more detail, similarly to the results presented in section 6.4. The results are presented and compared to the initial validation model run, originally presented in Figure 6-3, in Figure 7-3.

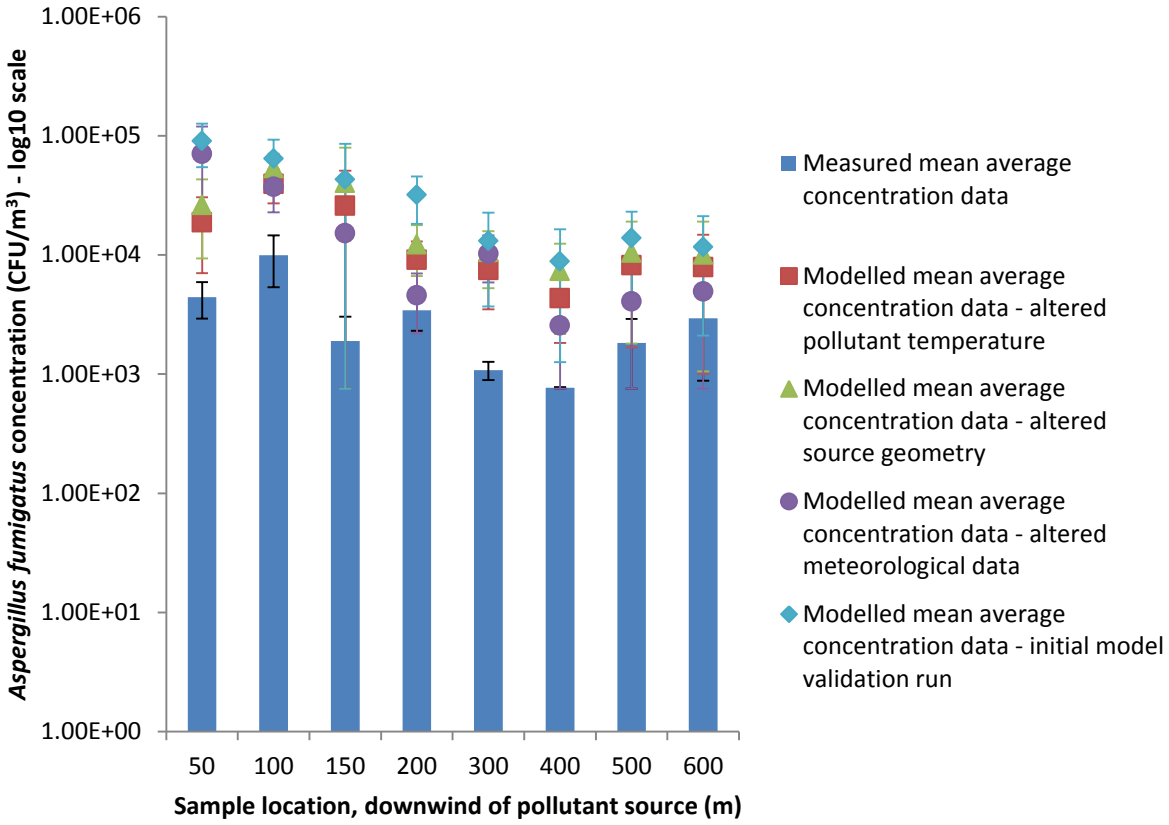

Figure 7-3 Validation results when altering selected model input values, compared to the initial model validation run. Black error bars denote the SEM of the sampled data, and the coloured error bars the SEM of the modelled data for: blue; the initial model validation run and when altering: red, pollutant temperature; green, source geometry; purple, meteorological data.

The most striking feature of Figure 7-3 is that all of the input parameter alterations have resulted in a reduced model output concentration. All alterations have also resulted in an overall change in the trend of the data, when compared to the initial model validation run. The overall trend of the data for the alterations in pollutant temperature and source geometry are the same, and mostly follows the trend of the initial model validation run, with the exception of the outputs at 50 and 200 metres downwind. The alterations in source geometry have resulted in the model overestimating the measured data more than when the pollutant temperature is altered, but still less than the initial model validation run. The meteorological data alteration has resulted in a more varied trend in the model output data, which does not appear to follow that of

the other model validation runs presented in Figure 7-3. This was somewhat anticipated, considering that the other model runs used the same set of meteorological data.

Table 7-4 presents the statistical analyses at each distance downwind of the emission source for the additional model tests, and compares them to the initial model validation, originally presented in Table 6-3.

Table 7-4 Statistics at each distance downwind of the source of emission for a) the original validation model run, originally presented in Table 6-3, and the additional model validation runs when altering 1) pollutant temperature 2) source geometry and 3) meteorological data. Any highlighted cells correspond to the limits presented in Table 5-3. '-' denotes a diving by 0 error when calculating the statistic.

Distance downwind (m)	Statistic											
	RMSE				EF				r			
	a)	1)	2)	3)	a)	1)	2)	3)	a)	1)	2)	3)
50	1004	739	1076	3128	-440.62	-105.25	-224.13	-1902.61	-0.33	0.06	0.07	0.11
100	835	1558	2235	1692	-28.68	-32.85	-68.66	-38.91	0.48	0.45	0.38	0.61
150	2809	2082	3313	1168	-2187.26	-1492.64	-3780.48	-469	1.00	1.00	1.00	1.00
200	879	610	884	337	-79.91	-62.12	-131.73	-18.28	0.32	0.61	0.59	0.57
300	2110	1585	2184	1895	-2465.42	-1549.82	-2942.16	-2215.56	0.73	0.84	0.83	0.34
400	1723	934	1873	629	-	-	-	-	-	-	-	-
500	866	618	857	245	-71.67	-36.01	-70.16	-4.81	0.99	0.99	0.99	1.00
600	406	293	424	125	-15.77	-6.94	-15.61	-0.45	0.99	0.99	0.99	1.00

Distance downwind (m)	Statistic											
	r^2				M				FB			
	a)	1)	2)	3)	a)	1)	2)	3)	a)	1)	2)	3)
50	0.11	0.00	0.01	0.01	-30831	-15303	-22750	-67151	-1.55	-1.38	-1.54	-1.81
100	0.23	0.20	0.15	0.37	-564844	-35333	-49109	-33143	-1.41	-1.62	-1.71	-1.60
150	1.00	1.00	1.00	1.00	75194	-24161	-38444	-13558	-1.82	-1.76	-1.84	-1.61
200	0.10	0.37	0.34	0.33	-11951	-7794	-10951	-3310	-1.27	-1.07	-1.27	-0.50
300	0.54	0.70	0.69	0.12	-10858	-6531	-9655	-9343	-1.67	-1.57	-1.68	-1.68
400	-	-	-	-	-5968	-3564	-6552	-1798	-1.59	-1.40	-1.62	-1.09
500	0.99	0.99	0.99	1.00	-8710	-6329	-8610	-2240	-1.41	-1.27	-1.40	-0.76
600	0.99	0.99	0.99	1.00	-7023	-5006	-7198	-2068	-1.09	-0.93	-1.11	-0.53

The statistics presented in Table 7-4 show that, generally, the correspondence between the modelled and sampled data:

- Improves when altering the pollutant temperature. Therefore these results suggest that the optimal input value of 29°C provided by the model calibration is appropriate when modelling *Aspergillus fumigatus* emissions at all open windrow composting facilities
- Worsens when altering the source geometry. These results indicate that the input used in the original model validation, 56.4 by8.4 metres, provided the best correspondence between the modelled and measured data, when applying the model to the Flixborough composting site. This parameter was originally altered from the optimal input provided by the model calibration, to represent the dimensions of a composting windrow, as detailed in Table 6-1. Therefore these results suggest that a site specific source geometry should be used to represent the area of a composting windrow at the facility that is being simulated
- Improves when altering the meteorological data. This was unexpected as these results suggest that meteorological data collected from a weather station located in close proximity to a different composting facility, provide the best fit between the modelled and the measured data. This notion is illogical and is discussed in section 7.5.2.

To summarise, the statistics presented in Table 7-4, indicate that when the pollutant temperature and meteorological data were altered to the optimal values provided by the model calibration OAT, the correspondence between the modelled and measured data improved. Therefore, these parameters were altered together to observe whether, together, it further improved the model fit with the sampled data. The statistical analysis confirmed that the fit between the modelled and sampled data was improved when these parameters were changed simultaneously (data shown as part of Table 7-5 and Figure 7-6). However, overall the fit between the modelled and sampled data, although improved, is not suitable enough to state that model has been successfully validated.

Ultimately, many model input parameter value alterations could have been tested. However, the alterations presented above were carefully justified to avoid performing a second model calibration. Despite this, the modelled outputs from all validation model tests have resulted in an overestimation of the measured data. Lowering the emission rate would help to overcome this issue, as the emission rate is directly proportional to the modelled output concentrations, when modelling without chemical or depositional effects (Johnson, 2011a). Therefore if the emission rate was decreased, then the modelled output concentration would also decrease. This hypothesis was tested, and is presented in section 7.4.

7.4 Emission rate alteration test

7.4.1 Approach

The sampled *Aspergillus fumigatus* data collected at Lount and Flixborough were compared. An optimal emission rate of $9x10^6$ CFU/m^2/s was provided by the model calibration, which was performed using data collected at Lount. If the concentrations of *Aspergillus fumigatus* collected at Flixborough were consistently lower than those collected at Lount, then this would justify a reduction in the optimal emission rate. The sampled data, collected at locations downwind of the site, are compared in Figure 7-4. The distances where the samples were collected at these facilities was not consistent. For example, at Lount, samples were collected at 50, 80, 100, 150, 180, 250, 280, and 300 metres downwind, and at Flixborough samples were collected at 50, 100, 150, 200, 300, 400, 500 and 600 metres downwind. Therefore the sampled *Aspergillus fumigatus* data is compared at the consistent locations, these being 50, 100, 150 and 300 metres downwind, in Figure 7-4.

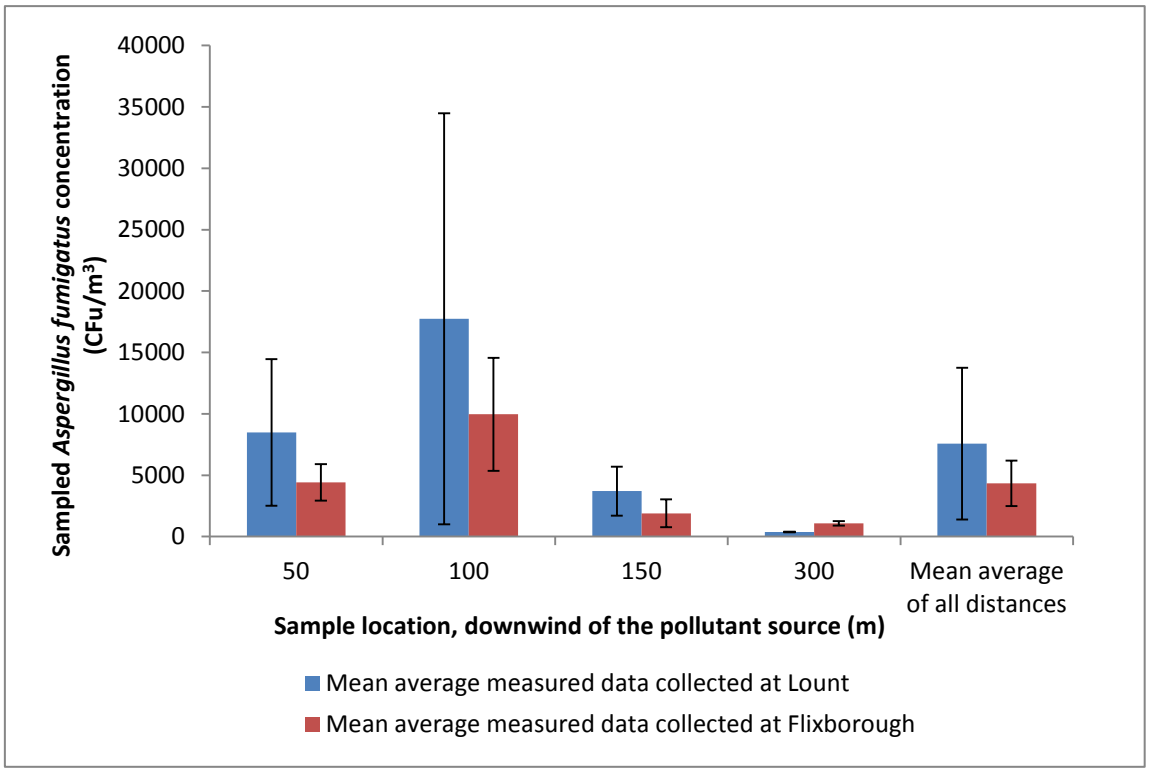

Figure 7-4. Comparison of the sampled data collected at Lount and Flixborough. Error bars denote the SEM of the mean averaged sampled data

It is appreciated that the measured data collected at Lount and Flixborough are statistically inseparable, as indicated by the overlapping SEM error bars in Figure 7-4. However, without considering the SEM, the mean averages of the measured data collected at Flixborough are consistently lower than the mean averages of the measured data collected at Lount, with the exception of the data collected at 300 metres downwind. This justifies the exercise of lowering the emission rate to test whether this will improve the correspondence between the modelled and the measured data.

The overall mean average *Aspergillus fumigatus* concentrations, at the common downwind distances, collected at Lount were 75% higher than the overall mean average concentrations collected at Flixborough. Therefore the optimal emission rate of $9x10^6$ CFU/m^2/s was reduced by this percentage to $2x10^6$ CFU/m^2/s. This emission rate is still within the range of emission rates

previously used within the dispersion models when simulating the composting scenario, as displayed in Table 2-6.

All other model inputs remained at the values used for the initial validation run as described in Table 6-1, with the exception of the pollutant temperature and meteorological data, which were altered according to the results of the additional model validation tests as discussed in section 7.3.2.

7.4.2 Results

A scatter plot comparing all of the modelled outputs with sampled data collected at downwind locations only is presented in Figure 7-5.

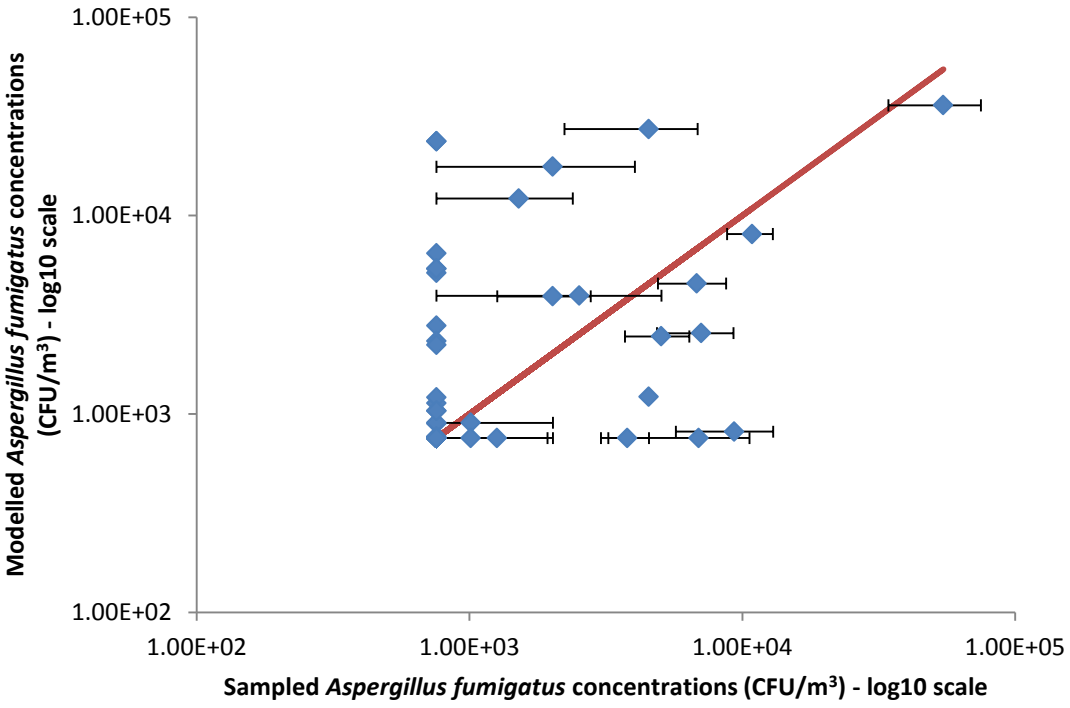

Figure 7-5 Scatter plot of the sampled data, collected at downwind locations, plotted against all modelled outputs using the altered emission rate. The error bars denote the SEM of the triplicated samples. The red line signifies where the points would fall if the modelled outputs corresponded perfectly to the measured values.

The results in Figure 7-5 are very different to the results of the initial model validation presented in Figure 6-2. The results in Figure 7-5 show that the

model is no longer predominantly overestimating the sampled the data. Similarly to the results presented in Figure 6-2, the modelled output and measured concentrations do not fall below 757 CFU/m^3, as previously explained. The statistical analysis of these results is presented in Table 7-5. For comparative purposes, Table 7-5 also presents the statistical results from the model validation which provided the best correspondence between the modelled and sampled data thus far, which was provided when modelling with the altered pollutant and meteorological data (data not previously presented).

Table 7-5 Statistics from the comparison the sampled data to the corresponding modelled outputs, at downwind locations for model validation 1) altered pollutant temperature and meteorological data 2) altered emission rate, pollutant temperature and meteorological data. Any highlighted values correspond to the limits presented in Table 5-3. All values presented are rounded to 2 decimal places.

Statistic	1) original emission rate, altered pollutant temperature and meteorological data	2) altered emission rate, pollutant temperature and meteorological data
RMSE	1056.57	258.20
EF	-12.88	0.17
r	0.60	0.60
r^2	0.36	0.36
F	40.16	40.16
M	-8429.14	-979.96
FB	-1.30	-0.35

The improved fit between the modelled and the sampled data when using he altered emission rate can instantly be observed in Table 7-5. The r and r^2 values appear to be identical for both model validation runs. This has occurred because the degree of association between the datasets, which is what the r statistic measures (Addiscott and Whitmore, 1987), has not changed by altering the emission rate. This is because the emission rate is directly proportional to the modelled output concentrations, when modelling without chemical or depositional effects (Johnson, 2011a), as previously stated. The fit between the

modelled and measured data at each distance downwind is illustrated in Figure 7-6, alongside the modelled outputs when altering the pollutant temperature and meteorological data only.

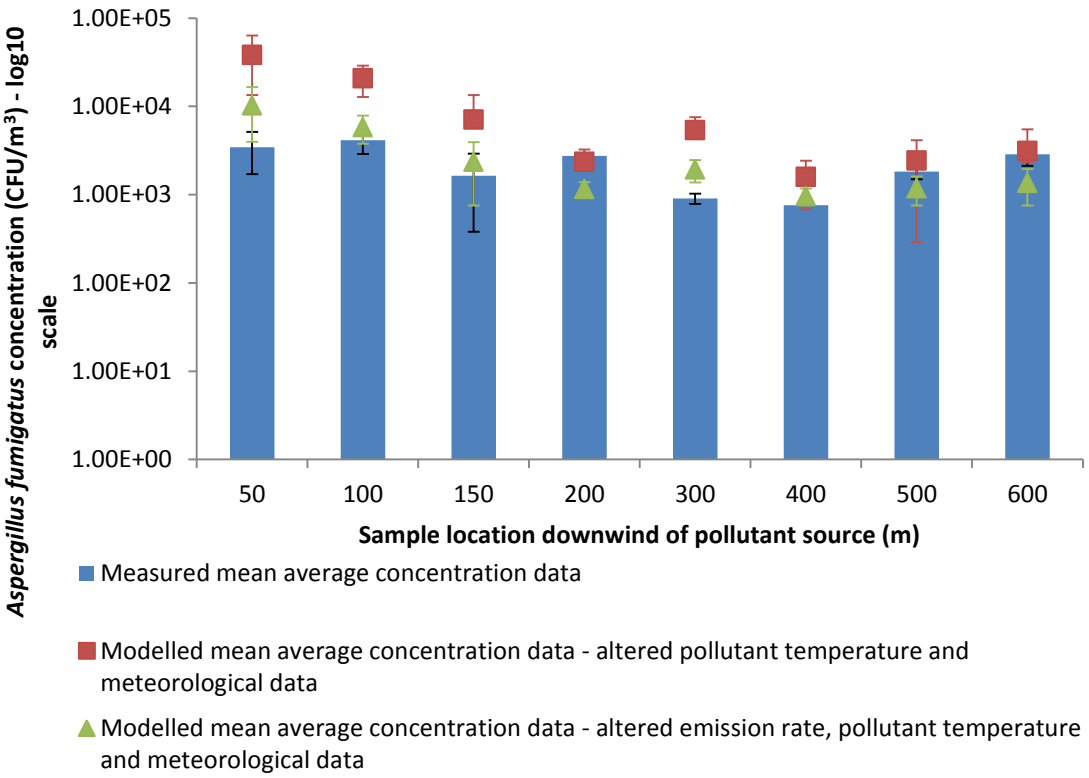

Figure 7-6 Results when modelling with altered pollutant temperature and meteorological data, with and without altered emission rate, at each distance downwind. Black error bars denote the SEM of the sampled data, the red error bars the SEM of the modelled data when altering pollutant temperature and meteorological data, and the green error bars the SEM of the modelled data when altering pollutant temperature, meteorological data and emission rate.

The results presented in Figure 7-6 show that altering the emission rate has improved the fit between the modelled and measured data. The model generally overestimates the measured data by less than one order of magnitude.

Table 7-6, presents the statistical results of the model runs using the altered pollutant temperature and meteorological data, with and without the adjusted emission rate, at each distance downwind of the emission source.

Table 7-6 Downwind location-specific statistics when altering 1) the pollutant temperature and meteorological data and 2) the pollutant temperature, meteorological data and emission rate. Highlighted cells correspond to the limits presented in Table 5-3. '-' denotes a diving by 0 error when calculating the statistic.

Distance downwind (m)	Statistic											
	RMSE		EF		r		r^2		M		FB	
	1)	2)	1)	2)	1)	2)	1)	2)	1)	2)	1)	2)
50	1613	377	-505.07	-26.58	0.07	0.07	0.00	0.00	-34921	-6814	-1.67	-0.99
100	863	213	-9.38	0.37	0.66	0.66	0.43	0.43	-16641	-1670	-1.34	-0.34
150	468	61	-74.48	-0.29	1.00	1.00	1.00	1.00	-5431	-710	-1.25	-0.36
200	109	37	-1.01	0.76	0.54	0.54	0.29	0.29	-1069	119	0.16	0.82
300	925	224	-526.81	-29.98	0.24	0.24	0.06	0.06	-4474	-1019	-1.42	-0.72
400	292	74	-	-	-	-	-	-	-834	-210	-0.71	-0.24
500	67	71	0.56	0.51	1.00	1.00	1.00	1.00	-614	648	-0.29	0.43
600	16	91	0.98	0.23	1.00	1.00	1.00	1.00	-271	1506	-0.09	0.71

Again, it can be observed in Table 7-6, that the r and r^2 values are identical for both model runs, confirming that changing the emission rate results in a proportionate change in the modelled concentration outputs. When observing all other values in Table 7-6, statistically the altered emission rate consistently improves the fit between the modelled and sampled data at distances up to and including 400 metres downwind. However, at 500 and 600 metres downwind, the statistics indicate that the fit between the modelled and sampled data is slightly worsened when modelled with the altered emission rate. Overall, altering the emission rate has improved the fit between the modelled and measured data.

7.5 Discussion

This chapter has presented the results of several model validation tests when using ADMS to simulate bioaerosol emissions from open windrow composting facilities. ADMS has never been tested in the open windrowcontext prior to the presentation of this thesis, and thus this chapter, and Chapter 6, has presented the first results of this novel application of the model. Statistical analysis has indicated that the ADMS dispersion model has not been successfully validated, as the correspondence between the modelled and sampled data does not meet the criteria detailed in Table 5-3, based on other model validation studies reported in the wider literature. However, the results of these additional validation studies have shown that the model is:

- Corresponding to the measured data more closely than when compared to the original modelvalidation results presented in Chapter 6
- Simulating *Aspergillus fumigatus* concentrations within one order of magnitude of sampled data

The best fit between the modelled and sampled data was achieved by:

- Not using the buildings options
- Using a pollutant temperature of 29.0°C, corresponding to the optimal value provided by the model calibration

- Using a site-specific source geometry, based on the length and width of a composting windrow on that site
- Using meteorological data collected from the closest weather station to Lount, and selecting the meteorological conditions at the dates and times at which the measured data was collected.
- Using an emission rate which is proportional to the measured concentration data

7.5.1 Comparison of results to previous modelling studies

Although the ADMS model has never been validated in the context of bioaerosol emission from open windrow composting facilities prior to this study, some previous studies have compared modelled results to some measured data. The few studies which have directly compared modelled outputs generated by ADMS to sampled *Aspergillus fumigatus* data are summarised below.

ADAS (2005)

ADAS (2005) used ADMS to model agitation activities from an open windrow composting facility. Emissions were represented as an area source, with a height of 1.8 metres and dimension of 2 by 10 metres. *Aspergillus fumigatus* concentrations were measured at 25, 75 and 125 metres downwind of the agitation activates and compared to modelled outputs. The raw modelled output data and sampled data were not provided, however, from graphical representations of the data, it was clear that the model had grossly underestimated the sampling data by more than 9 orders of magnitude. However, very low emission rates were used in the dispersion model ($6.0x10^{-6}$ $g/m^2/s$), which is the likely cause of this gross underestimation.

Drew *et al.* (2007)

Drew *et al.* (2007) modelled bioaerosol emissions from static windrows and agitation activities. Agitation activities were represented as 3 point sources, one for each type of agitation activity (turning, screening and shredding). Simple meteorological data was used, based on stability classes, and different

emission rates were used in the model, based on back extrapolations from measured data taken near the different agitation activities. As no raw data of the measured or modelled output values were presented in this study, model performance has been estimated from graphical representations of the data. Overall, the model underestimated the sampled data by 2 orders of magnitude.

SNIFFER (2007)

Similarly to Drew *et al.* (2007), bioaerosol emissions were estimated from agitation activities and static windrows. Again, a point source was used to represent emissions from agitation activities. From graphical representation of the data, it was apparent that the modelled outputs were underestimating the sampled data by more than 3 orders of magnitude.

Tamer Vestlund (2009)

Tamer Vestlund (2009) modelled *Aspergillus fumigatus* emissions from an open windrow composting facility located in Aberdeenshire, Scotland (Keenan Recycling). *Aspergillus fumigatus* concentrations were measured on two successive days at approximately 2 and 40 metres downwind of screening and shredding agitation activities, using SKC personal filter samplers. These measured results were compared to modelled outputs. The inputs used within the dispersion model included:

- Modelling the emission as a point source, with a height of 3 metres and diameter of 3 metres
- Using an emission rate of $7.5x10^5$ – $4.7x10^6$ CFU/s, back calculated from extrapolation
- Using meteorological data based on atmospheric stability classes (stability class D, constant wind speed and direction)

Graphical results indicated that the model underestimated the sampled data by less than one order of magnitude.

Overall, when comparing ADMS modelled outputs to sampled data collected at open windrow composting facilities reported in previous modelling studies, the

model has underestimated bioaerosol concentrations. In contrast to this study this study, where the model has generally overestimated bioaerosol concentrations by less than one order of magnitude. This study has also compared modelled outputs to a more comprehensive measured dataset. For example, modelled outputs have been compared to sampled data collected:

- At more sampling locations
- Over several different days
- Over different seasons
- During several agitation activities

7.5.2 Discussion of altered input parameters

The initial model validation run was performed with some model input parameters that deviated from the optimal model inputs, which were obtained by completing the model calibration. This was completed as it was originally thought that some site-specific model inputs would be required for the model to simulate conditions at the different site, Flixborough. The source geometry, pollutant temperature, meteorological data and grids data were altered from the optimal model inputs obtained through the model calibration. It should be noted that other site specific input parameter alterations were considered prior to validation, but alterations were not made. For example, the surface roughness model input value could have been changed to represent the surface roughness of the land surrounding Flixborough. The surface roughness model input parameter represents the land use type of the area surrounding the source of the pollutant emission (CERC, 2010b), which influences turbidity within the atmospheric boundary layer (Oke, 1987). Therefore the surface roughness of the land directly upwind of the site will determine the turbidity of the air on contact with the source of the pollutant. On inspection of the meteorological file, the wind direction was predominantly from the south-west. As illustrated in Figure 6-1, the land to the south-west of the facility is predominantly agricultural. Therefore the surface roughness was retained at 0.2 metres, representing agricultural land.

However, these site-specific alterations resulted in an overall poor fit between the modelled and sampled data. Therefore further tests were completed to observe whether the site specific alterations were improving or worsening the fit between the modelled and sampled data. Firstly, the use of the buildings options was tested (section 7.2), as the validation sampling site was located in close proximity to buildings whereas the calibration site was not, and thus this parameter was not tested during the model calibration. Secondly, the model input parameters were returned to their original optimal values, OAT (section 7.3). Finally, the emission rate was altered (section 7.4) in accordance to the differences in sampled concentrations of *Aspergillus fumigatus,* collected at the two measurement sites used in the model calibration and validation. The outcomes of these changes are discussed in this section.

7.5.2.1 Buildings module

Generally, when using the buildings options, the model overestimated the sampled data more than when the buildings options were not used. This difference was possibly observed because of how the model simulates air flow around a building. The presence of a building affects the boundary-layer flow and alters the dispersion of pollutants emitted from nearby source (Robins *et al.,* 2013). The effect of a building on air flow is illustrated in Figure 7-7.

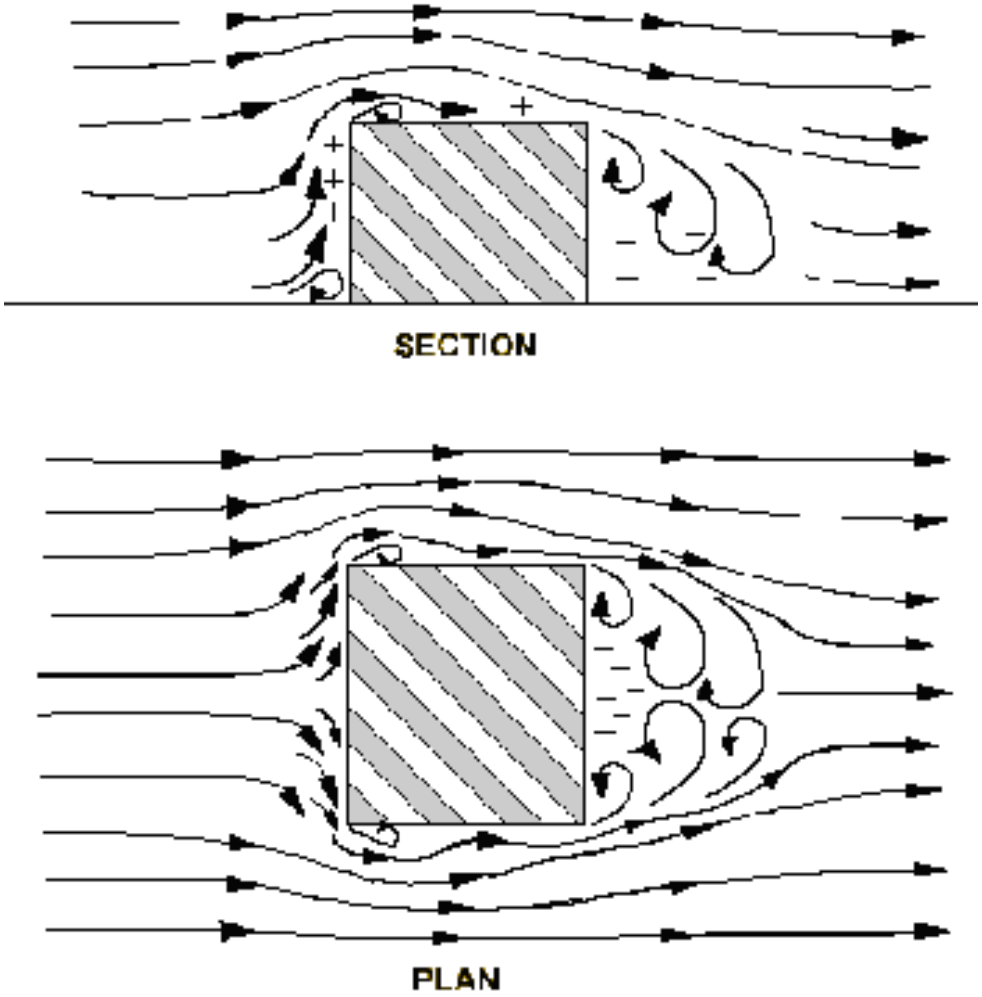

Figure 7-7 The effects of a building on air flow. Top – A cross-sectional view and Bottom – a plan view of air flow around a building (KAPER, 2005)

Figure 7-7 shows that the polluted air around the wake, or behind a building is recirculated. Effectively this entrainment decreases the dispersion of the pollutant, thus causing elevated concentrations of pollutants (Hayati and Sayadi, 2012; National Geographic, 2013b). Air around the building can be fully or partially entrained into the wake of the building (Robins *et al.,* 2013). This entrainment effect is simulated in ADMS, and thus is likely to have caused the slightly more elevated modelled concentrations observed when using the buildings options.

It is also possible that the use of the buildings option worsened the fit between the modelled and sampled data due to the input changes required in the model,

to allow the buildings options to be used (splitting a singular area source into 14 point sources as described in section 7.2.1).

7.5.2.2 Pollutant temperature

The correspondence between the modelled and measured data improved when the pollutant temperature was increased from 21.6°C to 29.0°C, indicating that a case-specific pollutant temperature is not required.This was unexpected for several reasons including the fact that:

- The pollutant temperature was discovered to be a slightly sensitive input parameter during the scenario specific sensitivity analysis (Chapter 4), and thus has a considerable effect on modelled output concentrations
- Initial measurements (presented in Chapter 8) indicated that the pollutant temperature was consistently higher than ambient temperature. As ambient temperature is highly variable, it was also thought that the pollutant temperature would also be highly variable

It is widely understood that warmer air is less dense than cooler air, causing it to ‘rise’; occasionally this is referred to as thermal rise, buoyancy rise or thermal buoyancy (Beychok, 1994; Barratt, 2001). Therefore an increased pollutant temperature results in an increased difference between the pollutant temperature and ambient temperature, causing an increase in pollutant plume rise (Beychok, 1994; Barratt, 2001). Consequently it takes longer for the pollutant to descend to breathing height levels, and allows more time and space for the pollutant to disperse, resulting in decreased pollutant concentrations. This is conceptualised in Figure 7-8, and accounts for the differences between the two model runs displayed in Figure 7-3.

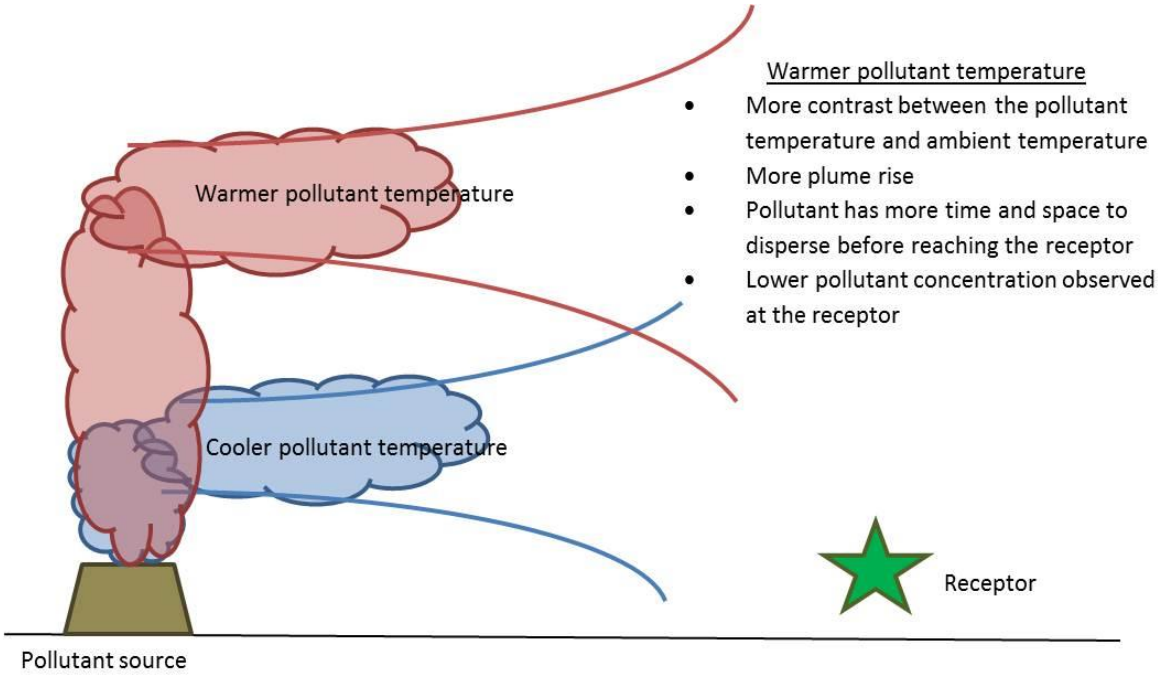

Figure 7-8 Conceptualisation of the effect of the altered pollutant temperature on modelled output concentrations, based on information from Beychok (1994) and Barratt (2001). The blue plume represents the cooler pollutant temperature used in the initial model validation run, 21.6°C and the red plume the warmer pollutant temperature used in the altered validation run, 29.0°C.

7.5.2.3 Source geometry

Results indicated that a source geometry specific to the site being modelled, based on the area of a composting windrow, is required to provide the best fit between the modelled and sampled data.This is unsurprising when considering the sensitivity of this parameter (Chapter 4).

The source geometry used in the initial model validation run, which provided the best fit, was 56.4 by8.4 metres, which is longer and narrower than the altered source geometry of 44.0 by9.5 metres. The longer and narrow source geometry resulted in an overall decrease in modelled output concentration, but worsened the fit between the modelled and the sampled data. A decrease in the modelled output concentration was expected, due to the way that the model simulates area sources. The model user guide (CERC, 2010b) states that each source is decomposed into a maximum of 10 source elements. Source elements which

do not significantly contribute to pollutant concentration at the receptor are disregarded. This is partially dependant on the alignment of the source to the predominant wind direction, as illustrated in Figure 7-9.

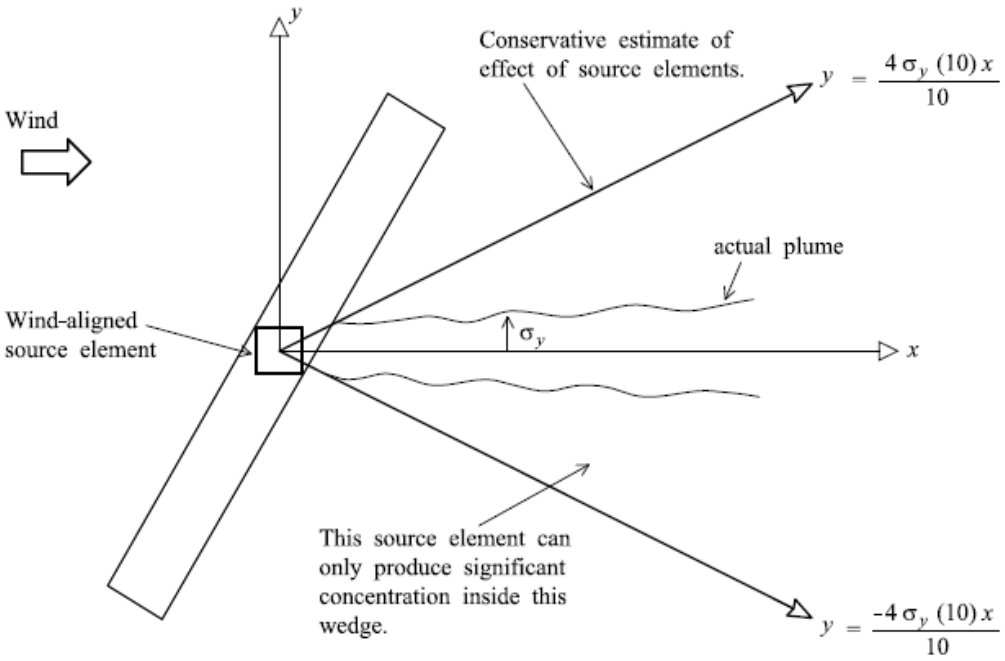

Figure 7-9 Effects of area source orientation and predominant wind direction on pollutant dispersal. Where x is the downwind distance from the source (m), y is the lateral distance from the source (m) and σ_y is the plume dispersion parameter in the horizontal direction (m). Taken from CERC (2010b).

It can be seen in Figure 7-9 how the orientation of the area source, or more specifically, the area source element, with the predominant wind direction can affect the extent of σ_y, the plume dispersion in the horizontal direction. When observing the Gaussian equation, Equation 2-1, it is clearly shown that larger values of σ_y will result in lower pollutant concentrations. Therefore the orientation of the area source element with the predominant wind direction effects the pollutant concentration. The predominant wind direction when modelling the effects of the different source geometries remained constant, as the same meteorological data was used in both model runs. However, as previously stated the source geometries did alter. A higher modelled output

concentration, and statistically improved fit between the modelled and measured data, was observed with longer and narrower source geometry. By applying the principles illustrated in Figure 7-9 to the geometries modelled in this chapter, it can be easily shown why a higher modelled output concentration was observed when a longer and narrower source was used, as shown in Figure 7-10.

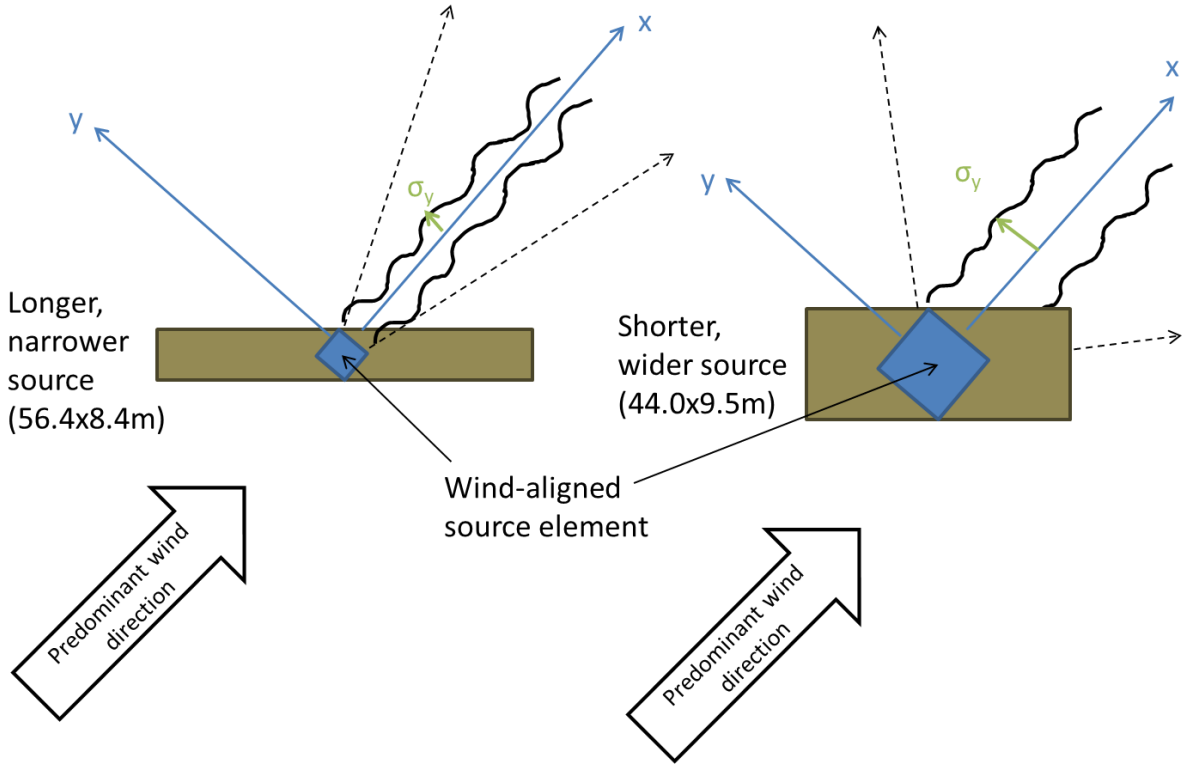

Figure 7-10 Application of information presented in Figure 7-9 to the source geometries tested in this chapter (not to scale). Where x is the downwind distance from the source (m), y is the lateral distance from the source (m) and σ_y is the plume dispersion parameter in the horizontal direction (m). Adapted from CERC (2010b).

It can be clearly seen in Figure 7-10 that by modelling with longer narrower source geometries results is smaller values of σ_y. As previously stated, smaller σ_y values result in higher modelled output concentrations, which correspond to the results observed in this chapter, and highlights the sensitivity of this model input parameter. Therefore small changes in the source geometry will result in

large changes in the model outputs, and thus it is vital that the correct source geometry and source orientation is used within the dispersion model.

7.5.2.4 Meteorological data

It has been long established that meteorological conditions are a major factor in determining the dispersion of air pollutants (Oke, 1987; De Nevers, 2000). Therefore it was expected that changing the meteorological input would have an effect on the modelled outputs. What was unknown was whether this change would improve or exacerbate the fit between the modelled and measured data. All meteorological data used throughout the validation tests was purchased from the UK Meteorological Office (Met Office, 2011a). Initially, data collected from the closest weather station to Flixborough was used in the model. Using this data produced modelled outputs that did not correspond well to the measured data, although the outputs followed the general trend of the measured data, as depicted in Figure 6-3. The optimal inputs derived from the completion of the model calibration used meteorological data collect from the weather station located closest to Lount. This meteorological data was applied to Flixborough to investigate what input parameters were causing the poor fit between the modelled outputs and the measured data. The alteration in the meteorological data did produce a statistically improved fit between the modelled and sampled data. These results indicate that using meteorological data collected from a weather station located closest to another composting facility, in this case Lount, provide the best fit between the modelled and the measured data. This notion is abstract, as this suggests that data collected from a meteorological station located closest to another composting facility provides improved modelled outputs when simulating emissions from a different site. To explore this further, the two meteorological datasets are compared. To reiterate, two datasets were used during the model validation:

1) Data collected at the nearest weather station to Flixborough, selecting data at the times and dates that sampling occurred at Flixborough, was used in the initial validation model run.

2) Data collected at the nearest weather station to Lount, selecting data at the times and dates that sampling occurred at Flixborough, was used in the altered validation model tests.

These meteorological datasets are now referred to as 1)F, and 2)LF respectively. To reiterate, modelling with meteorological data 2)LF provided the best fit between the modelled and the measured data. The meteorological data used in 1)F and 2)LF were collected from the weather stations Leconfield and Sutton Bonington respectively. Leconfield is located approximately 34 kilometres north east of Flixborough, and located 2 kilometres north of the nearest town, Beverley in East Yorkshire. Sutton Bonington is located approximately 15 kilometres north east of Lount and 93 kilometres south west of Flixborough. The nearest town to Sutton Bonington is Kegworth, located 2 kilometres east of the weather station. Both weather stations are located a long distance from the closest composting facility, although Leconfield is located just over twice as further from Flixborough than Sutton Bonington is to Lount. The local meteorology at the weather stations will be different to the meteorology at the composting facilities. Local meteorology, sometimes referred to as micro-scale meteorology, signifies meteorological conditions observed at small scales and is an important factor in the dispersal of pollutants (Chang *et al.,* 2006; Howard and Naini, 2012). Both weather stations are located in rural locations with relatively flat terrain, and thus do not present any major topographical complexities. However, Flixborough is located in a topographically complex location, as described in section 6.2, and is positioned in close proximity to many large buildings and a major river, the River Trent. Therefore Flixborough will experience different local meteorology than that measured at Leconfield, the closest weather station to the composting facility. Laković *et al.* (2012) reported the importance of local meteorological effects on pollutant emissions from coal-fired power plants. This study reports how weather conditions have influenced how the power plant is operated to ensure that the site complies with environmental limits. The importance of local meteorology may explain why meteorological data collected at Lount resulted in an improved fit between the modelled and measured data when simulating *Aspergillus fumigatus* emissions

at Flixborough. The properties of the meteorological data sets used through the validation are compared in Table 7-7, by means of basic statistical calculations. This will assess the main differences between the meteorological datasets, which will help to apportion the causes of the differences between the observed modelled output concentrations.

Table 7-7 Comparison of the meteorological datasets used within the model validation

Meteorological input (units)	Statistic	Meteorological file	
		1) F	2) LF
Wind speed (m/s)	Range	0.514–10.289	0.100-4.633
	Mean	4.244	2.766
	Median	3.858	3.089
	Mode	2.572	4.118
Wind direction (º)	Range	10-330	10-360
	Mean	227	243
	Median	250	250
	Mode	250	250
Temperature (ºC)	Range	2.2–18.6	2.2-19.7
	Mean	9.9	10.6
	Median	9.4	10.0
	Mode	8.8	8.5
Relative humidity (%)	Range	53-100	46-100
	Mean	78	78
	Median	76	78
	Mode	100	100
Cloud cover (oktas)	Range	0-8	0-8
	Mean	5	6
	Median	7	7
	Mode	8	8

It is clear in Table 7-7 that the main difference between the two meteorological datasets is the wind speed. The wind speed range in 1) F includes much higher wind speeds. This indicates that the wind speed element within the meteorological data files has been the major cause of the differences observed

between the modelled output concentrations when altering the meteorological data. This coincides with the findings of the Pankhurst (2010), who attempted to analyse the impact of meteorological conditions, measured at the composting facility, on bioaerosol concentrations. Pankhurst discovered that wind speed had a significant effect on *Aspergillus fumigatus* concentrations at both Lount and Flixborough. Wind speed was also discovered to be sensitive during the screening stages of the sensitivity analysis (chapter 3), although the level of sensitivity of this parameter was not quantified.

Overall, the process of altering the meteorological data within the dispersion model has highlighted the importance and sensitivity of this parameter when modelling bioaerosol emissions from open windrow composting facilities. This shows that it is vital that good quality meteorological data is used within the dispersion model when simulating the open windrow composting scenario. However, if using meteorological data collected from weather stations outside of the local metrological 'zone' of the site (~>10km) then care should be taken when using this data, particularly if the topography between the weather station and composting facility differ. Ultimately, the most accurate meteorological data that could be used within the dispersion model would be collected at the composting facility where the bioaerosol emissions are being modelled. The collection of on-site meteorological conditions is recommended in the AfOR sampling protocol (AfOR, 2009).

7.5.3 Limitations

As the validation chapter has applied similar approaches and model inputs used in the model calibration, the limitations stated within Chapter 5, in section 5.5.3, also apply here. However there was a limitation specific to the model validation, associated with the use of the buildings option.

The principal limitation of the buildings model is associated with the way the source is represented. The results of the model calibration suggested that the source be represented as an area. However, area sources cannot be used when modelling buildings, and thus had to be converted into a series of point sources. This required alterations in the source dimensions and source

emission rate, which are both sensitive parameters, as discovered in Chapter 4. Again this will have affected the model output concentrations. However the limitations of these two buildings issues were reduced as much as possible by following the recommendations of the ADMS model developers (Lad, 2012b). Additionally, the model is only capable of simulating the turbulent effects around convex buildings. Therefore non-convex buildings were enlarged to rectangular shape. This may have altered the simulated turbulent effects around the buildings and thus the modelled output concentrations. To overcome this limitation it would be possible to divide a non-convex building into a series of convex shapes. However, this is unlikely to be effective as the ADMS model simplifies a series of buildings into a singular complex (Robins *et al.,* 2013), and thus was not tested. When these limitations within the model have been addressed by the model developers, CERC, then the buildings options should be re-tested.

7.6 Conclusions

An open windrow compositing specific model validation was performed on the ADMS model for the first time, utilising the optimal inputs provided by the model calibration. Selected model input parameters were adjusted to test whether site-specific model inputs were required when applying the model to different open windrow composting facilities. The tests indicated that the best fit between the modelled and sampled data was achieved by:

- Using a pollutant temperature of 29.0°C, corresponding to the optimal value provided by the model calibration
- Using a site specific source geometry, based on the length and width of a composting windrow on the site being modelled
- Using a site specific emission rate
- Not using the buildings options

These results provide modellers with improved parameter input values, and with enhanced insights of how to represent the source of the emission in this scenario. Statistically the modelled data did not correspond to the measured

data. However the modelled data did not over or underestimate the data by more one order of magnitude. This has improved on all previous modelling attempts when simulating the open windrow composting scenario. However, further modelling tests are required to confirm or disprove these results, and to improve the model performance.

The next chapter describes the progress made when attempting to quantify some of the model input parameters using novel measurement techniques.

8 Model input parameter measurements

8.1 Introduction

The ADMS model has been rigorously tested in the specific scenario of modelling bioaerosol emissions emitted from open windrow composting agitation activities, by completing a sensitivity analysis [SA], Chapters 3 and 4, and model calibration and validation, Chapters 5, 6 and 7. This chapter utilises and builds on the findings from these chapters. It should be noted that the work presented in this chapter was carried out alongside the work presented in Chapters 3, 4, 5 6 and 7. Therefore the emerging results of those chapters informed the work in the chapter and vice versa.

Chapter 2 highlighted that past attempts of modelling bioaerosol emissions from composting facilities were not successful, and model outputs did not correspond well to measured values. An analysis of those previous studies revealed that the measurement or estimation made for several model input parameters was generally not stated or justified. Therefore it can be assumed that many of these model inputs were speculative. However, it should be recognised that there was limited datasets to use within these studies. It is very likely that this lack of knowledge and data surrounding several of the input parameters within the model is accountable for the lack of success in modelling bioaerosol emissions from open windrow composting facilities to date. The objective of this chapter is: 'to collect data, using novel techniques and existing data collection methods if possible, to improve the knowledge of selected dispersion model inputs, in the open windrow composting context, to provide more accurate modelled output concentrations'.

Several model inputs were discovered to be sensitive in Chapter 4, these included:

- The wet and dry deposition modules
- Majority of inputs associated with the source of the emission

Due to time constraints, it was not possible to improve the quantification of all of the sensitive model inputs. Therefore the improvements were prioritised to the

parameters of which there are fewer existing measurements. As the model was calibrated and validated with moderate success without the need to adjust the wet and dry modules or the pollutant molecular mass input, improved quantification of these parameters has not been completed at this stage. Source geometry estimates have been made with some justification in the past (Millner *et al.,* 1980; Taha *et al.,* 2006) and can be estimated using objective and systematic protocols based on observations and using technical specifications of the machinery used to agitate the compost. Similarly thesurface roughness can be estimated using the land-use options available within the ADMS model (CERC, 2010b). Pollutant temperature and pollutant exit velocity cannot be estimated with confidence and therefore attempts to improve the quantification of these parameters are made in this chapter. Prior to this study, it was known that the emission rate is a sensitive input parameter (Johnson, 2011a). The results from the model validation also suggested that a site-specific emission rate is required to allow bioaerosol emissions from open windrow composting facilities to be modelled with greater accuracy. The parameters required to calculate an emission rate during agitation activities include: pollutant concentrations at source, pollutant exit velocity and source dimensions. As already stated, source dimensions can be estimated using systematic methods and attempts to quantify the pollutant exit velocity are made in this chapter. However, it has not yet been possible to collect bioaerosol concentrations at the source of agitation activities due to health and safety constraints (Taha *et al.,* 2006). Therefore this chapter describes the novel approach used to collect bioaerosol concentration data at the source of the agitation activities. Consequently, preliminary emission rate calculations, based on the measurements completed in this chapter are also presented.

The improved model input parameter measurements and calculations completed within this chapter can be used in future model runs, along with any other parameter quantifications that may also be completed in the future, to allow more realistic model inputs and thus outputs.

8.2 Prior art

Existing modelling studies, reviewed in Table 2-6, have attempted to model bioaerosol emissions from composting facilities. This section summarises the key findings of these studies in respect of the pollutant temperature, pollutant exit velocity and pollutant emission rate model inputs.

8.2.1 Pollutant temperature

As highlighted in section 2.5.3, two studies (Drew *et al.,* 2005; Tamer Vestlund, 2009) justified the pollutant temperature used within a dispersion model when simulating bioaerosol releases from composting facilities. Drew *et al.* (2005) and Tamer Vestlund (2009) used the measured ambient temperature as the pollutant temperature input within the dispersion model. As previously discussed, the pollutant temperature is thought to be above ambient temperature, as composting cores can reach up to and beyond 55-60°C (Lacey and Crook, 1988). Tamer Vestlund (2009) considered this, and modelled a 'high pollutant temperature' scenario using a value of 55°C. However, it is also thought that the pollutant temperature will be lower than the compost core, as the hot core is exposed to the cooler ambient air, allowing the hot air, and any pollutants contained within it to rise, disperse and cool rapidly on release. This is illustrated in Figure 2-4. Therefore, at present there are no known measurements or reliable estimations of the temperature of bioaerosol emissions from agitated compost windrows. Turner *et al.* (2005) used a Thermal Imaging Camera [TIC] to measure the surface temperature of a composting heap to determine pathogen inactivation. A similar method is described in section 8.4.1, whereby a TIC has been used to quantify the temperature of bioaerosols (the pollutant) at the time of release during open windrow composting agitation activities (the source of emission) for the first time. A TIC forms images using infrared radiation. On a basic level TICs work like a common camera, but within the infrared wavelength range, not the visible wavelength range. A TIC can be used at a safe distance from agitation activities, ensuring operator safety. TICs are used in many contexts including

surveillance, law enforcement and security, building diagnostics and optical gas imaging (FLIR, 2012a).

8.2.2 Pollutant exit velocity

Only three studies have stated what pollutant exit velocity was inputted into the dispersion model. Drew *et al.* (2005), Taha *et al.* (2007) and Tamer Vesltund (2009) modelled with pollutant exit velocities ranging between 0.19 and 1.70 metres per second, although it was not justified why these values were used. Therefore it has been assumed that the pollutant exit velocity has been estimated in the past, as there are no known measurements or justified estimations of the pollutant exit velocity at composting facilities.

During stack releases, the pollutant exit velocity can be easily measured using anemometers across the area of the stack (SNIFFER, 2007). Anemometers are used to measure wind speed, or the velocity of any current of gas (National Geographic, 2013a). It would be difficult to use anemometers to measure the pollutant exit velocity from composting agitation activities because:

- Emissions from composting facilities are sporadic and are not contained. Therefore correct positioning of an anemometer would be difficult, particularly as anemometers need to be positioned perpendicular to the plane of the pollutant emission to allow accurate velocity readings (Omega, 2012)
- Sampling near agitation activities is impractical and dangerous (Taha *et al.,* 2006)

Section 8.5 describes the preliminary pollutant exit velocity estimations made by observing plume movements between fixed points, using video camera footage.

8.2.3 Pollutant emission rate

A large range of pollutant emission rates, covering several orders of magnitude, have been previously used within dispersion models, as highlighted in Table 2-6. Pollutant emission rates are usually estimated by back extrapolation using bioaerosol concentrations sampled at distances of at least 2 metres downwind

of the agitation activity (Danneberg *et al.,* 1997; Dowd *et al.,* 2000; Environment Agency, 2001b; Taha and Pollard, 2004; ADAS, 2005; Taha *et al.,* 2006; Taha *et al.,* 2007; SNIFFER, 2007). There are many limitations to back extrapolation as highlighted in section 2.5.1, and thus emission rates derived from measurements may be more accurate than emission rate estimation via back extrapolation.

Current data cannot be used to calculate an emission rate. As pollutants disperse and dilute immediately upon release (Beychok 1994), a bioaerosol concentration measured at 2 or more metres downwind of the point of emission would not be appropriate for calculating an emission rate.

At present it has not yet been possible to measure bioaerosol concentrations at the point of emission using existing sampling methods, due to the dangers associated with sampling near to agitation activities (Taha *et al.,* 2006). Section 8.6 describes the novel technique used to sample bioaerosol concentrations during agitation activities within 0.3 metres of the point of release. To calculate an emission rate, knowledge of the pollutant exit velocity and geometry of the emission is also needed. Thus the methods and results of the improved quantifications of pollutant temperature, pollutant exit velocity and pollutant concentration at source are presented first, followed by resulting emission rate calculations.

8.3 Site descriptions

Sampling was completed at three sites in total. Pollutant concentration and pollutant exit velocity measurement improvements were completed at one site only, due to the strict health and safety procedures put in place to allow the completion of the work possible. Pollutant temperature measurements were completed at three sites. Due to the nature of the equipment availability, sampling visits were often planned at short notice, and thus sampling was completed at any site that was able to accommodate this.

8.3.1 Amey Cespa

AmeyCespa (East) waste facility, now referred to as Amey Cespa, is located on the A10 approximately five miles north of Cambridge and is rural in location. This site was used to complete all bioaerosol concentration and exit velocity measurement improvements. The nearest sensitive receptor is the IQ business park, located approximately 400 metres south east of the site. There are also some farm buildings situated within 1 kilometre of the site boundary. The site contains a Mechanical Biological Treatment [MBT] plant, open and in-vessel composting areas, landfill, recycling services and areas where waste, including construction and demolition waste, can be transferred or dropped off (AmeyCespa, 2012). Sampling was performed on the open windrow composting sections of the site only. The site produces approximately 12,000 tonnes of organic waste, including household garden waste, and commercial green waste (AmeyCespa, 2012). The composting process takes approximately 12 weeks. The site is well managed, having gained BSI PAS 100 accreditation (AmeyCespa, 2012). Windrows are kept moist, and odours are controlled with neutralisers. The site is in operation between 0800 and 1700 hours Monday to Friday, and 0800 and 1200 hours on a Saturday. For health and safety purposes, all sampling was carried out on a Sunday when the site was closed, as described in more detail in section 8.6.2.2.

8.3.2 Ramsey

AWO Recycling Limited, now referred to as Ramsey, is located near Ramsey Heights in Cambridgeshire. Like Amey Cespa, the site is rural in location. The nearest sensitive receptors are the residents of Ramsey Heights, Upwood and Ramsey located 1-2 kilometres South East, South and East of the site. The site is small in comparison to AmeyCespa only processing green garden waste. The site does not accept any cooked food waste or animal by-products (AWO Recycling Services, 2008). The composting process takes at least 8 weeks and the compost is turned at least 4 times, more so at the beginning of the process (AWO Recycling Services, 2008). Like AmeyCespa, this site has also gained BSI PAS 100 accreditation (AWO Recycling Services, 2008). Materials are well

blended to minimise odour emissions, and windrow temperatures are checked daily (AWO Recycling Services, 2008). The site is in operation between 0730 and 1730 hours Monday to Friday, and 0800 and 1200 hours on a Saturday. The site is closed on a Sunday.

8.3.3 Fields Farm

CRJ Recycling, now referred to as Fields Farm, is located near Sandbach in Cheshire. The site, again, is rural in location, with the nearest receptors 1-2 kilometres away in the villages of Ettiley Heath and Wheelock, North and East of the site respectively. Like Ramsey, the site is small, and processes only green waste (CRJ, 2010). Only one activity is carried out at a time when necessary, due to the limited numbers of operators working at the site. Like Ramsey and AmeyCespa, the site is well managed, having gained BSI PAS 100 (CRJ, 2010).

8.4 Pollutant temperature quantification

8.4.1 Method

Thermal imaging cameras [TICs] were borrowed from the EPSRC instrument pool. Three thermal imaging cameras were borrowed in total over the sampling period, dependant on availability. A summary of the technical specifications of each camera used is provided in Table 8-1. All cameras were portable and powered by battery.

Table 8-1 Thermal imaging camera technical specifications.

	Camera model		
	SC 3000	E45	T400
Spectral range (µm)	8.0-9.0	7.5-13.0	7.5-13.0
Thermal Sensitivity	20mK	100mK	50mK
Temperature ranges (°C)	-20 – 2000	-20 – 250	-20 – 120
Accuracy (°C)	±1	±2	±2
Resolution (pixels)	320 x 420	160 x 120	320 x 240
Other info	Stirling cooled to 70 Kelvin. Autofocus	-	Able to capture infrared videos. And thermal fusion images
References	FLIR™ (2000)	FLIR™ (2006)	FLIR™ (2011)

Table 8-1 states the camera specifications for thermal sensitivity and accuracy. Thermal sensitivity relates to the resolution of the thermal images [TIs] produced by the camera. Cameras with low sensitivity are able to produce more detailed TIs, with clearer temperature differences (ICI, 2013). The accuracy relates to the error of the apparent temperature reading formed by the camera.

As seen in Table 8-1, the three cameras have different specifications. This does cause slight discrepancies between the temperature readings that each TIC would give. Moreover, there would even be slight discrepancies between duplicated models due to manufacturing tolerances (Anthony, 2013). The extent to which these discrepancies alter TIC readings is highlighted in Table 8-2, which compares the calibration tables of each TIC model.

Table 8-2 Comparison of the calibration tables for each TIC model (FLIR™, 2012a; FLIR™, 2012b; FLIR™, 2012c)

Camera model	Reference temperature (°C)	TIC temperature reading (°C)	Difference between the reference temperature and the TIC temperature reading (°C)
SC3000	21.70	21.10	0.60
E45	22.38	22.90	0.52
T400	21.80	21.60	0.20

Table 8-2 shows that each TIC model results in a slightly different temperature reading when compared to a reference temperature. The difference between the temperature readings of each TIC is less than 1°C, and thus the discrepancies between the TIs taken with the different TIC models will be less than 1°C.

The TICs were used like an ordinary camera. The camera was assembled on a tripod and placed approximately 5-10 metres from the agitation activities. The camera was focussed and programmed to take images every 2-10 seconds. The camera was used to capture the temperature of the pollutant plume during turning, screening and shredding activities. As recommended by the ITC (2009), the TIC was used, where possible:

- at an angle perpendicular to the activity, to avoid any thermal reflection
- in a position where there were no other activities being carried out in the background of the image, to avoid misinterpretation when analysing the images

The FLIR™ T400 camera was capable of taking TIs alongside regular images [RIs] within the visible light spectrum, and able to capture video footage. TIs were captured mainly in winter months when ambient temperatures were expected to be low in an attempt to capture maximum contrast between the pollutant plumes and the background atmosphere. Ambient temperatures were measured using a Kestral® weather station (Kestral® 3000, Nielsen Kellerman, USA).

An emissivity value of 0.96 was used within the thermal imaging camera. Emissivity is the ratio of the radiation emitted by an object when compared to a perfect emitter of radiation, or blackbody (ITC, 2009). Emissivity values can fall within a range of 0 to 1: 1 represents a perfect blackbody, and 0 represents a perfect reflector of radiation (EOI, 2013). If an incorrect emissivity is used, it can result in inaccurate temperature readings. It is assumed that the observed plume of dust and steam also contains bioaerosols. As the pollutant plume is opaque and thus likely to be unreflective, a high emissivity was expected (Batty, 2010), however, preliminary tests were completed to determine what emissivity setting should be used. Two objects of known emissivity, one high and one low were placed in front of a compost windrow. A red brick and a piece of aluminium with an emissivity of 0.93 and 0.40 respectively were used. A temperature probe was used to measure the temperature of the pollutant plume during compost turning, and was placed as close to the agitation activity as possible, without causing harm to the sampler. The ambient temperature was also recorded. The emissivity setting on the TIC was adjusted to that of the materials of known emissivity. It was noted that the lower emissivity resulted in un-realistic temperature readings; for example a measurement of -20.0°C was recorded, when the ambient temperature was 23°C. This confirmed that a higher emissivity was needed. Therefore the emissivity was adjusted until the temperatures measured by the TIC corresponded to those measured by the temperature probe. Theoretically, a temperature probe could have used as an alternative method to a TIC when quantifying pollutant emission temperatures. It was decided that this method would not be used as it can only provide a spot temperature measurement in space and time whereas a TIC can capture larger areas and can be used continuously. A TIC is also easier and safer to use, as it allows the sampler to measure temperatures at a safe distance from the agitation activities.

Like emissivity, the reflected apparent temperature [RAT] is also an important input within the TIC. Thermal energy from other objects may be reflected from the target object, in this case the pollutant plume, into the TIC affecting the TIC

reading (MII, 2010). As the pollutant plume is opaque, and assumed to be quite unreflective, the RAT was set to 0.

Images were analysed using FLIR QuickReport© (1999-2013) software. Emissivity and RAT settings can be altered post-measurement within this software. Image analysis was completed under the advice of the ITC (2009). Prior to analysis, as the camera was set up to take images every 2 -10 seconds, all images that did not capture agitation activities were disregarded. All images analysed were captured no more than 30 seconds after an agitation activity. Within the FLIR QuickReport© software, the relative humidity, ambient temperature and the distance the camera was positioned from the emission was entered. The temperature range and span was altered to give the clearest image. The 'RainHi' colour palette was used to give maximum temperature contrast, although this may also be altered post-analysis. The area tool was used to provide the maximum and minimum temperatures of the pollutant plume. It was not possible to analyse all images due to poor image resolution or due to lack of pollutant plume visibility on the TI.

8.4.2 Results

Figure 8-1 shows an image taken with the T400 TIC during a turning activity. This image is shown alongside a RI. The images were taken at Ramsey. The ambient temperature on the day of the measurement was 10.6°C, which is depicted as a black colour within the thermal image.

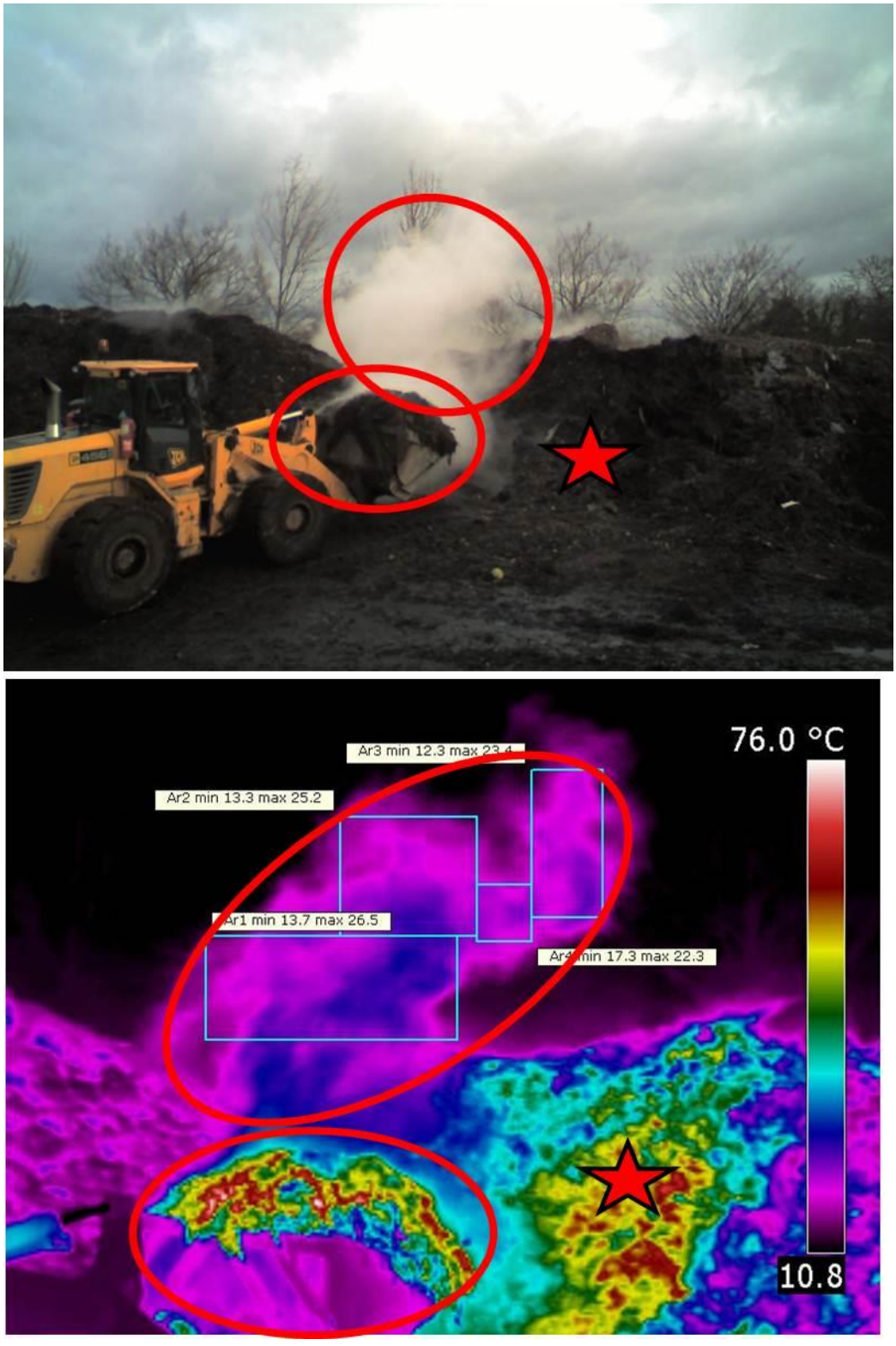

Figure 8-1 A RI (top) taken alongside a TI (bottom) of a turning activity using the T400 TIC. The images have been annotated to highlight corresponding areas. Results of the analysis of the pollutant plume using the area tool in FLIR QuickReport© are also displayed on the thermal image. Personal photographs.

The TI in Figure 8-1 shows significant plume rise, caused by the effects of the exposure of the hot compost core to cooler ambient temperatures, as conceptualised in Figure 2-4. The windrow core exposure is highlighted with a red star within the images presented in Figure 8-1. This image was captured approximately 5 seconds after material was removed from a windrow during a turning agitation. It can be observed that the pollutant plume temperature decreases on distance from the agitation activity, as depicted by the blue to purple colour change in the TI. Figure 8-1 shows areas drawn across the pollutant plume using the area tool in FLIR QuickReport© on the TI. The maximum and minimum plume temperatures observed in this particular image were 26.5 and 12.3°C respectively, represented by the blue and purple colours in the image correspondingly. This gives a difference of 1.7-15.9°C between the ambient temperature and the pollutant plume temperature.

Unfortunately, it was not possible to capture as many TIs during screening and shredding activities, due to site operations on the day of measurements. However it was possible to capture these activities with the TIC at least once. A TI taken during a shredding activity with the T400 TIC at Amey Cespa is presented in Figure 8-2. THe ambient temperature on the day that this image was taken was 3.6°.

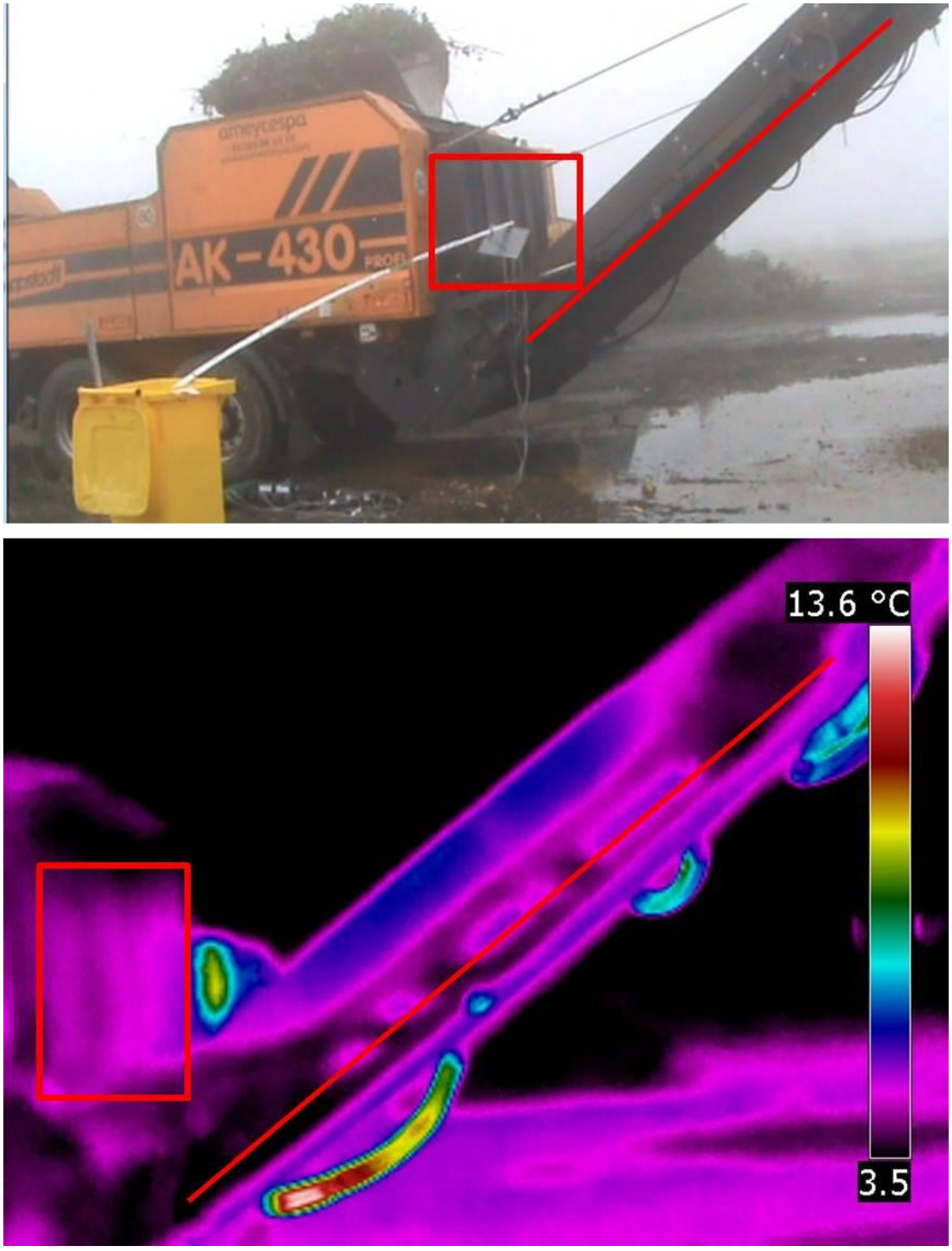

Figure 8-2 A RI (top) taken alongside a TI (bottom) of a shredding activity using the T400 TIC. The images have been annotated to highlight corresponding areas. Results of the analysis of the pollutant plume using the area tool in FLIR QuickReport© are also displayed on the thermal image. Personal photographs.

Figure 8-2 shows that the shredding activity does not cause a pollutant plume, as there is no evidence of a pollutant plume present on the TI. Therefore it was not possible to analyse this image. The image was captured on the same day as the TI shown in Figure 8-1, and thus the ambient temperature is the same

Unfortunately, it was not possible to capture screening activities with the T400 TIC, due to camera availability and site operations on the day of measurement. Therefore it was not possible to take RIs alongside TIs. Figure 8-3 shows a TI taken during screening activities, alongside a RI taken at a similar angle, but not at the same time as the TI. The RI has been displayed for ease of depiction of the key features in the TI, and not for direct comparison.

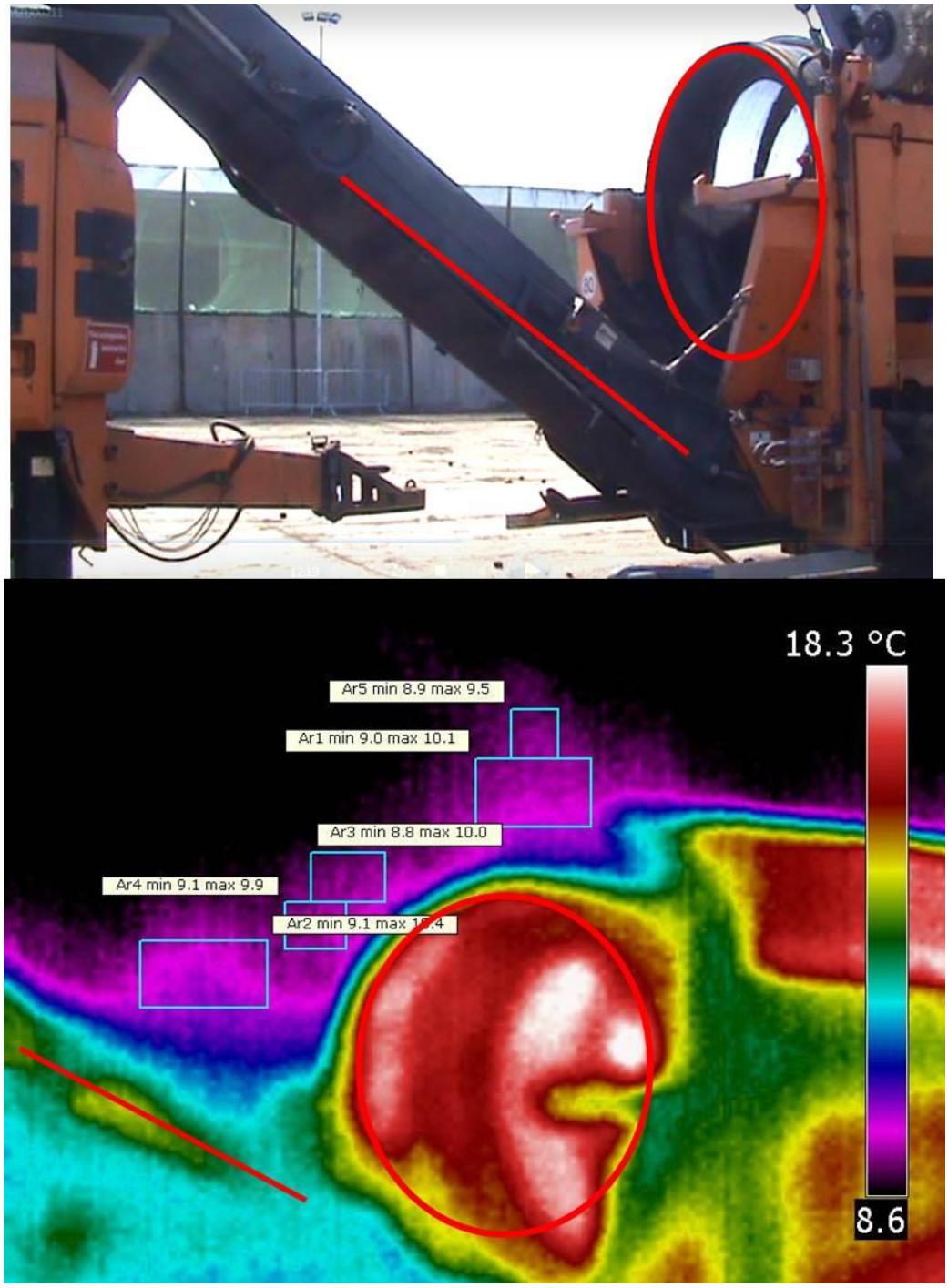

Figure 8-3 A RI (top) taken at a similar angle but at a different time to a TI (bottom) of a screening activity. Please note that as these images were not taken at the same time, the RI is displayed for TI interpretation only. The images have been annotated to highlight corresponding areas. Results of the analysis of the pollutant plume using the area tool in FLIR QuickReport© are also displayed on the thermal image. Personal photographs.

The TI presented in Figure 8-3 was taken using the E45 TIC at Amey Cespa. The ambient temperature on the day of measurement was 8.6°C, as depicted by the black colour in the TI. The pollutant plume is depicted as a purple colour in the TI. Some plume rise can be seen in the TI in Figure 8-3, although when compared to the turning activity in Figure 8-1, the appearance of the plume rise does not seem to be as effective. Again it can be observed that the temperature of the pollutant plume decreases upon emission. The maximum and minimum temperatures of the TI obtained from area analysis within FLIR QuickReport©, were 10.4 and 8.8°C respectively. This is a difference of 0.2 to 1.8°C when compared to the ambient temperature, which is lower than the turning activity.

A summary of all of the pollutant plume temperatures measured using the TICs via analysis in FLIR QuickReport© are displayed in Table 8-3.

Table 8-3 Summary of pollutant plume temperatures measured with TICs during agitation activities. Images were analysed in FLIR QuickReport©. 'PR' denotes that that the images could not be analysed due to poor resolution, and 'NP' denotes that the images could not be analysed due to lack of presence of a pollutant plume. 'AC' refers to Amey Cespa

Date	Site	Activity	TIC used	Ambient temperature [AT] (°C)	Minimum temperature(s) of pollutant plume [MinT] (°C)	Maximum temperature(s) of pollutant plume [MaxT] (°C)	MinT - AT (°C)	MaxT - AT (°C)
13/01/11	Fields Farm	Turning	SC3000	9.0	9.4 – 12.5	15.5 – 22.6	0.4 – 3.5	6.5 – 13.6
02/02/11	AC	Turning	E45	11.6	12.1	18.0	0.5	6.4
12/01/12	Ramsey	Turning	T400	10.6	11.1 – 12.3	24.6 – 29.6	0.5 – 1.7	14 – 19
29/01/12	AC	Turning	T400	3.6	3.7 – 5.8	5.3 – 13.5	0.1 – 2.2	1.7 – 9.9
27/05/12	AC	Turning	SC3000	23	PR			
17/01/11	AC	Shredding, (indoor)	SC3000	4.5 (outside)	NP			
29/01/12	AC	Shredding	T400	3.6	NP			
02/02/11	AC	Screening	E45	8.6	8.8 – 9.0	10.4 -10.6	0.2 – 0.4	1.8 – 2.0
27/05/12	AC	Screening	SC3000	23	NP			

Table 8-3 shows that of those images analysed, the pollutant plume observed remained higher than ambient temperature. A difference of up to 19°C between the ambient temperature and measured pollutant plume temperature was observed. The difference between the minimum and the maximum observed pollutant temperatures are quite broad, indicating that the pollutant plume cools rapidly immediately after release. As indicated in Table 8-3, some images could not be analysed as a pollutant plume was not visible in the TI. This occurred on three occasions. Addressing each occurrence individually:

- The TI of shredding activities taken on the 17th of January 2011 (17/01/11) at Amey Cespa were captured indoors. It is assumed that the indoor ambient temperature was higher than the ambient temperature outdoors, and therefore the lack of plume presence may have been caused by the lack of temperature contrast between the pollutant plume and the warmer ambient indoor air
- TIs of shredding activities on the 29th of January 2012 (29/01/12) at Amey Cespa were captured outdoors on a cool day but still did not yield a visible pollutant plume. As shredding activities are completed on relatively new waste, that has not been subjected to the heating of the compost windrow during the more advanced phases of composting, shredding activities may simply not be hot enough to produce a pollutant plume
- The TIs of screening activities on the 27th of May 2012 (27/05/12) at Amey Cespa were captured on a hot day, with ambient temperatures of 23°C. Therefore it may be possible that there was not enough contrast between the ambient temperature and the pollutant plume temperature to produce a visible pollutant plume

Some thermal videos were also captured using the T400 TIC, but it is not possible to analyse thermal videos quantitatively. However it was still possible to observe pollutant plumes with higher than ambient temperatures released from the composting agitation activities. During turning activities it was observed that pollutant plumes were released for approximately 30 seconds after

agitation. Pollutant plumes were also observed during screening activities, but were emitted more continuously and appeared to be less vigorous than the turning activities. No pollutant plumes were observed in the TIC videos taken during shredding activities.

In summary:

- In all of the TIs that were analysed, the temperature of the pollutant plume was higher than the ambient temperature
- Shredding activities did not yield a measurable pollutant plume
- Turning activities appeared to be hotter, more vigorous and more sporadic than screening activities
- The temperature of the pollutant plume decreased rapidly upon release, and all pollutant plumes observed were subjected to plume rise

8.5 Exit velocity - preliminary quantification

8.5.1 Method

A camcorder (SONY® Handycam DCR-SR35E) was set up to record the movements of the pollutant plume released during agitation activities. Ambient wind speeds were recorded using a Kestral® weather station (Kestral® 3000, Nielsen Kellerman, USA). The exit velocity was estimated based on the time taken for the pollutant plume to move between two fixed points, or rods. Ideally the two rods would have been placed horizontally at a known vertical distance to allow the estimation of the vertical velocity of the pollutant plume, at the source of the emission. However this was impractical so close to the source of the agitation activity. Therefore the rods were placed at a measured distance vertically to estimate the horizontal velocity of the pollutant plume instead. This is clarified in Figure 8-4. Figure 8-11 illustrates this measurement technique in practise.

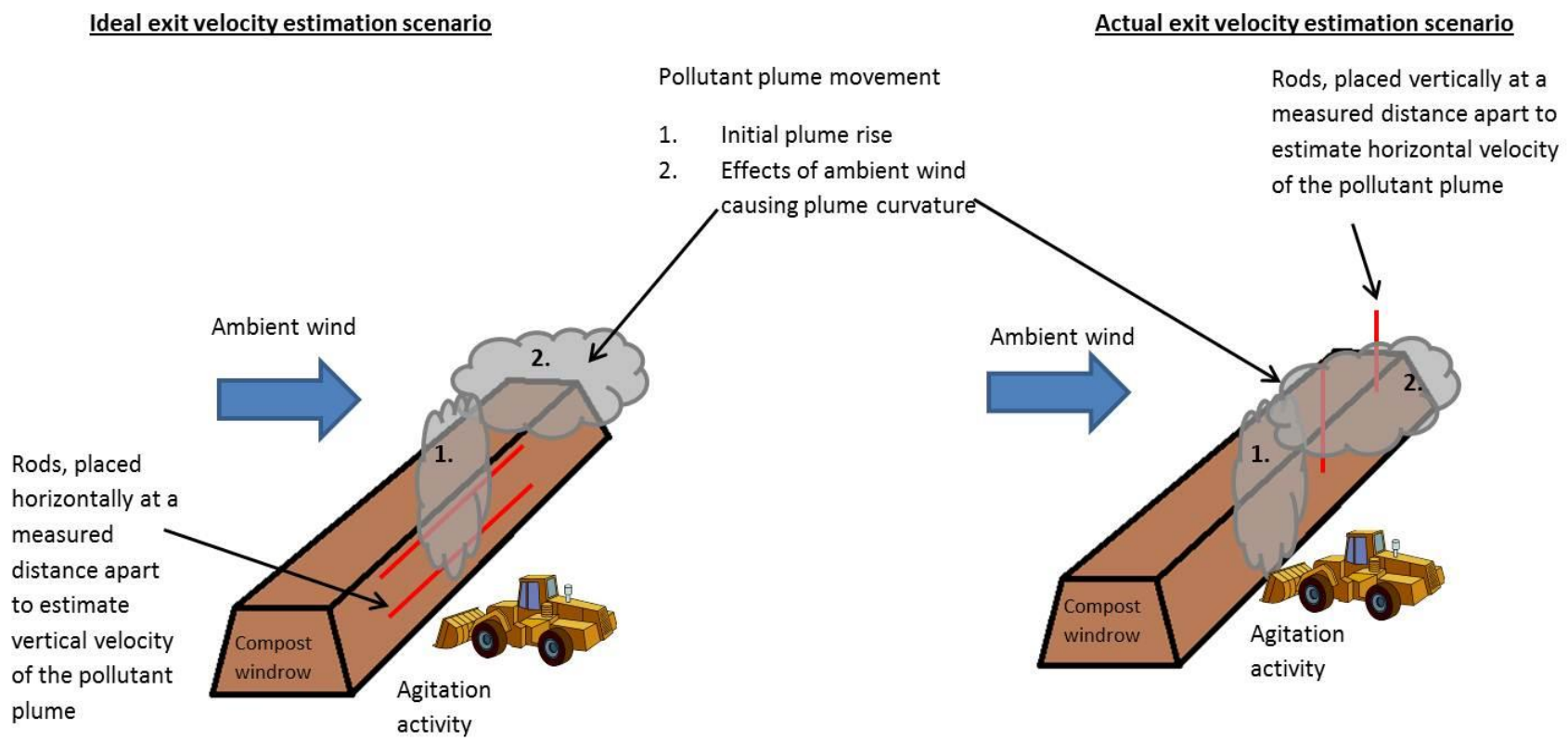

Figure 8-4 Illustration of the ideal (left) and actual (right) methods of estimating the pollutant exit velocity

If it was not possible to place the rods close to the source of the agitation activity, the distance between two fixed points was measured instead.

On some sampling occasions it was possible to record the pollutant plume movements using the T400 TIC as detailed in section 8.4. However, it was not feasible to use these recordings to estimate a pollutant exit velocity because it was not possible to predict how far the pollutant plume had travelled, as the fixed points were not visible on the thermal video.

After on-site sampling, the videos were observed, and a pollutant exit velocity was estimated using Equation 8-1.

$$V = \frac{D}{T}$$ **Equation 8-1**

Where:
V is the pollutant exit velocity in metres per second
D is the distance travelled by the pollutant plume in metres
T is the time taken by the pollutant plume to travel distance D in seconds

8.5.2 Results

Results of the estimated pollutant exit velocities are presented in Table 8-4. It was not possible to estimate the pollutant exit velocity from every sampling occasion as the pollutant plume was not always visible, and thus these occasions are not presented in Table 8-4.

Table 8-4 Estimated pollutant exit velocities estimated by observing pollutant plume movements captured on video camera

Date	Site	Activity	Ambient wind speed (m/s)	Estimated pollutant exit velocity (m/s)
02/02/11	Amey Cespa	Turning	1.6	1.5
06/11/11	Amey Cespa	Turning	5.0	3.0
06/11/11	Amey Cespa	Screening	3.5	2.0
29/01/12	Amey Cespa	Screening	0.6	0.3
06/11/11	Amey Cespa	Shredding	Shredding was performed indoors	0.5

Table 8-4 shows that the estimated pollutant exit velocities vary from 0.3 to 3 metres per second. The measured ambient wind speed was consistently above the estimated pollutant exit velocity.

8.6 Quantification of bioaerosol concentrations at source

To calculate the pollutant emission rate, a pollutant concentration at source is required. This section describes the novel technique used to sample within approximately 30 centimetres of agitation activities, to improve the quantification of bioaerosol concentrations at source.

8.6.1 Sampling strategy

Prior to sampling, turning, screening and shredding activities were observed to determine optimal sampling locations when attempting to characterise these emissions. The sampling strategies suggested below were based on these initial observations.

8.6.1.1 Turning

Turning agitation activities were performed using a Volvo L-series front end loader [FEL] (Volvo, 2009). It was observed that the turning activity consisted of material being removed from an existing windrow and moved to form a new windrow. Therefore turning activities with a FEL consists of three actions, as illustrated in Figure 8-5:

1. Removing material from existing windrow A
2. Transportation of the material
3. Depositing the material to form new windrow B

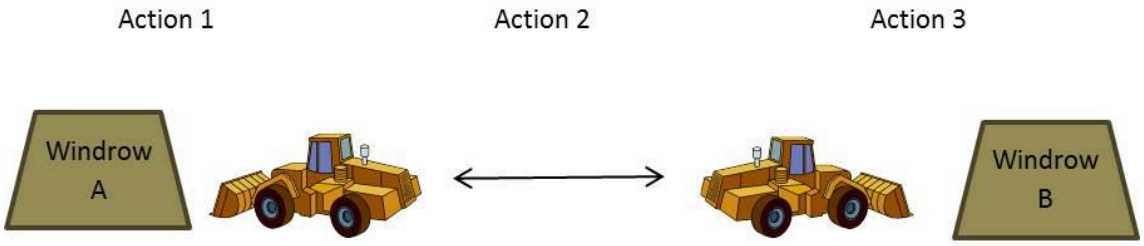

Figure 8-5 A profile illustration of the typical actions performed during turning activities with Front End Loader [FELs] (not to scale)

It was also observed that there were considerable dust and steam emissions, and therefore presumed elevated bioaerosol emissions, during actions 1 and 3. It was assumed that bioaerosol emissions were negligible throughout action 2, as dust and steam emissions subsided rapidly after actions 1 and 3. Subsequently, when attempting to characterise the bioaerosol concentrations at the source of this activity, sampling was completed to capture actions 1 and 3. To enable safe sampling within close approximation of the turning activity, the sampling equipment, as illustrated in Figure 8-6, was set up at the opposite side of the windrow to the activity. This allowed the equipment to be positioned over the windrow to within centimetres of the agitation activity on the other side. It was also ensured that the sampling equipment was set up in a downwind position from the activity. When sampling this activity, concentrations from a windrow approximately half way through the composting process were measured.

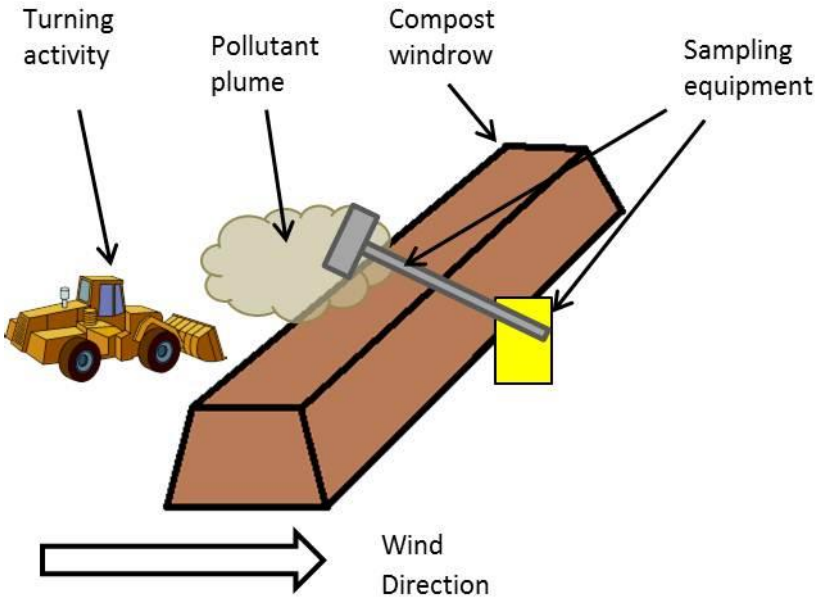

Figure 8-6 Illustration of how the sampling equipment was positioned during agitation activities whilst maintaining sampler safety (not to scale)

8.6.1.2 Shredding

Shredding agitation activities were performed using a Doppstadt AK series grinder (Doppstadt, 2009a). It was observed that the shredding activity consisted of placing material into the shredder and then removing it to form a windrow at the end of the shredding process. This was considered to be a series of seven actions, as illustrated in Figure 8-7:

1. Removing material from the newly arrived waste pile A, using a FEL
2. Transporting the material to the shredding machine
3. Depositing the material into the shredder inlet
4. Newly shredded waste exiting the shredding machine via a conveyor belt to form a pile of shredded waste, B
5. Removing material from shredded waste pile B, using a FEL
6. Transportation of the material
7. Depositing the material to form new windrow C

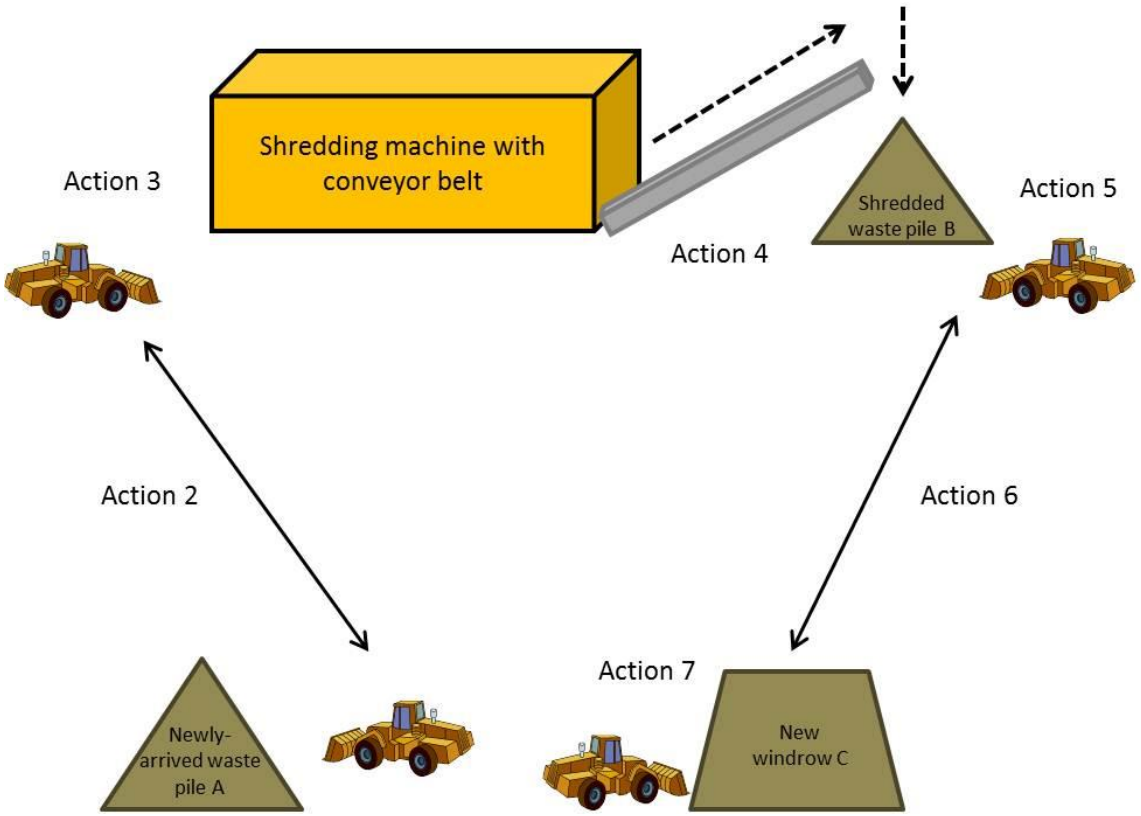

Figure 8-7 Illustration of the typical actions performed during shredding activities (not to scale)

Comparing the actions completed during turning and shredding, as illustrated in Figure 8-5 and Figure 8-7 respectively, it can be seen that there are some similarities between the two actions. Turning action 1 is similar to shredding actions 1 and 5. Turning action 3 is similar to shredding actions 3 and 7. However it should be recognised that the age of the compost during the turning activities is older than the compost agitated in the shredding activities, and thus the biological components of the compost at these two stages will differ (Swan *et al.,* 2003). However, it was not possible to sample the effects of the age of compost due to due to time and equipment constraints.. Like turning action 2, it was assumed that bioaerosol emissions were negligible throughout shredding actions 2 and 6. Therefore, only shredding action 4 is significantly different from the turning actions. Consequently, when attempting to characterise the bioaerosol concentrations at the source of this activity, sampling was completed to capture action 4, as it was considered that actions 1, 3, 5 and 7 were characterised when sampling turning activities. To ensure safety of the sampler,

the equipment was set-up similarly to the turning activity as illustrated in Figure 8-6, whereby the equipment was positioned near to the shredding equipment in a downwind position.

Additional safety factors were also implemented when sampling this activity. As the grinding machinery is loud and is subject to displacing material during operation, the sampling equipment was set up when the shredding machine was not in operation. Once the equipment was in place, the pumps were set on a delayed timer for five minutes. During the five minutes, the shredding machine was started whilst the sampler moved away from the machinery to a safe area.

8.6.1.3 Screening

Screening agitation activities were performed using a Doppstadt SM series screen (Doppstadt, 2009b). Screening activities are quite complex, as more vehicle movements are involved because the material is sorted into different sizes. This was considered to be a series of eleven actions, as illustrated in Figure 8-8:

1. Removing material from windrow A, using a FEL
2. Transporting the material to the screener
3. Depositing the material into the screener

Screener sorts the material into two size grades: a coarse fraction and a fine fraction. The coarse fraction is:

4. Transported via a conveyor belt to form a pile of coarse waste, B
5. Material is removed from pile B using a FEL
6. Material is transported
7. The material is deposited back to form a new windrow, or incorporated into an existing windrow, C

The finer fraction is:

8. Transported via a conveyor belt to form a pile of fine waste, D
9. Material is removed from pile D using a FEL
10. Material is transported
11. The material is deposited to form a new pile, E, to be bagged and/or sold as compost

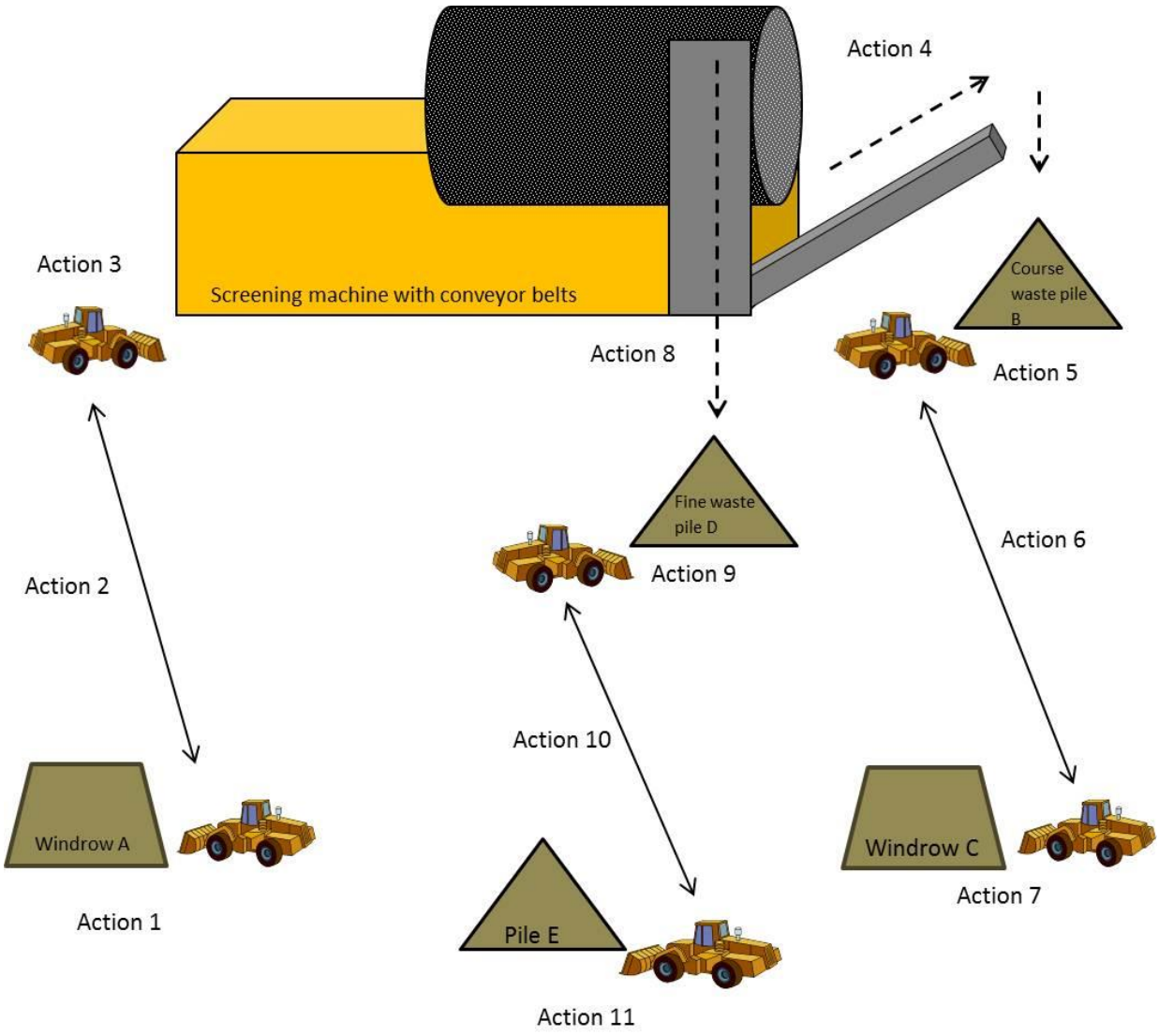

Figure 8-8 Illustration of the typical actions performed during screening activities (not to scale)

Like the shredding activity, there are many similarities between the screening activity and the turning activity as illustrated in Figure 8-8 and Figure 8-5

respectively. Turning action 1 is similar the screening actions 1, 5 and 9. Turning action 3 is similar to screening actions 3, 7 and 11. Like turning action 2, it was assumed that bioaerosol emissions were negligible throughout screening actions 2, 6 and 10. Therefore these actions were considered to be characterised by sampling the turning activities. Again, it should be noted that the age and thus biological components of the compost will differ, but this is not considered at this stage (Swan *et al.,* 2003). Screening actions 4 and 8 are similar to shredding action 4, as illustrated in Figure 8-7. However it was not assumed that the sampling of the shredding activities could be applied to the screening activities because:

- The screening and shredding activities represent the very beginning and the very end of the composting process, and are therefore completely contrasting
- The composition of the material is very different. Fresh waste is used during shredding whereas soil-like compost is screened

Consequently screening agitations 4 and 8 were also characterised and sampled. Due to the close approximation of these actions, the actions were combined into a singular sampling event, when attempting to characterise the source of the screening agitation activity. At the sampling site, two screeners were used in series to sort the material into different grades of compost, during normal operations. However, as not all sites use multiple screeners, and for simplicity, only one screener was in operation when sampling this agitation activity.

8.6.1.4 Sampling strategy summary

Table 8-5 summarises the agitation activities described in sections 8.6.1.1, 8.6.1.2, and 8.6.1.3.

Table 8-5 A summary of the agitation activity actions for each agitation activity type described in sections 8.6.1.1, 8.6.1.2, and 8.6.1.3. 'N/A' indicates not applicable.

Movement	Agitation activity		
	Shredding	**Turning**	**Screening**
Material transportation	Actions 2 and 6	Action 2	Actions 2, 6 and 10
Material removal	Actions 1 and 5	Action 1	Actions 1, 5 and 9
Material deposition	Actions 3 and 7	Action 3	Actions 3, 7 and 11
Material exit from shredding machine	Action 4	N/A	N/A
Material exit from screening machine	N/A	N/A	Actions 4 and 8

Sampling was completed at four sampling locations:

- Shredding action 4
- Turning action 1
- Turning action 3
- Screening action 4/8

These are now referred to as shredding, turning removal, turning deposit and screening respectively.

8.6.2 Sampling method

Where possible the AfOR standard protocol for monitoring bioaerosols at open windrow composting facilities (AfOR, 2009) was used. The sampling methods used are similar to those carried out by Tamer Vestlund (2009) and Pankhurst (2010), whereby sampling was completed using SKC personal aerosol filter samplers (SKC Inc, 2012).SKC samplers were used, as highlighted in section 2.3.3 and in Pankhurst (2010) because:

- High concentrations of bioaerosols can be collected
- Samples can be taken over short or long time periods

- The sampling equipment is light, easily transportable and simple to use
- Sample replication is relatively inexpensive and straightforward

All samples were collected at Amey Cespa. Aseptic techniques were carried out where necessary. If required, equipment and solutions were sterilised in an autoclave for 15 minutes at a temperature of 121ºC unless otherwise stated.

8.6.2.1 Pre-sampling preparation

Three bioaerosols were cultured, *Aspergillus fumigatus,* Gram-negative Bacteria and Total Bacteria, using selective agars. The AfOR protocol (2009) requires that *Aspergillus fumigatus* and Total Bacteria are measured on-site. Therefore the selective medias, Malt Extract Agar [MEA] and Nutrient Agar [NA] were used to culture *Aspergillus fumigatus* and Total Bacteria respectively, as described in the protocol, (AfOR, 2009). Although not a requirement, the protocol suggests that Gram-negative Bacteria should also be monitored, (AfOR, 2009; Environment Agency, 2009a); MacConkey agar [MAC] (Oxoid) was used to selectively culture Gram-negative Bacteria. Descriptions of media preparation for *Aspergillus fumigatus* and Total Bacteria are provided in the standardised protocol (AfOR, 2009). MAC was prepared by dissolving 52 grams of MacConkey agar powder for every litre of deionised water. The agar was then sterilised. Once cooled to approximately 47ºC, 0.1 grams of cycloheximide per litre was added aseptically to prevent fungal growth. Approximately 20 millilitres agar was poured under aseptic conditions into sterile 90 millimetre Petri dishes. Once set the agar plates were wrapped and refrigerated for no longer than a week until required. To allow samples to be suspended and diluted, a buffer solution was also prepared. Deionised water was sterilised at 121ºC for 15 minutes. Once cooled, 1 gram of salt and approximately three drops of Tween 80 were added per litre of sterile water under aseptic conditions. SKC sampling heads, filters and cassettes were also sterilised, and wrapped in foil to maintain sterility when transporting equipment to site.

8.6.2.2 On-site sampling

Prior to sampling, a camcorder (SONY® Handycam DCR-SR35E) was set up to record site activities. Weather conditions were also recorded using a Kestral®

weather station (Kestral® 3000, Nielsen Kellerman, USA). If necessary a thermal imaging camera, as discussed in section 8.4, was also set-up. SKC personal samplers (SKC Inc., 2012) were used whereby air is sucked through a filter, and any bioaerosols in the air are captured on the filter. Any bioaerosols captured on the filter are suspended in a sterile buffer solution to allow processing in the laboratory, as explained in sections 8.6.2.1 and 8.6.2.3. Polycarbonate filters with a diameter of 25 millimeters and pore size of 0.8 microns were used. Sterile filters in cassettes were placed into IOM sampling heads and attached to pumps via Tygon® tubing. All pumps were calibrated prior to sampling so that air was extracted at a rate of 2 litres per minute. To avoid contamination of samples, gloves were worn and cleaned with 70% ethanol prior to handling. Work was carried out swiftly to avoid unnecessary exposure in air. Figure 8-9 illustrates how the sampling heads were set-up and used. Samples collected during screening and turning activities were taken in sextuplet, with a blank, and samples collected during shredding activities were taken in triplicate with a blank. Ideally samples taken during shredding activities would have been taken in sextuplet, but this was not possible due to equipment constraints. Three sampling trips were completed in total in Autumn, Winter and Spring, in an attempt to capture any seasonal variability. A sampling time of 2 minutes was used as established by Tamer Vestlund (2009) when sampling bioaerosols in the immediate proximity of composting agitation activities simulated in a rotating drum

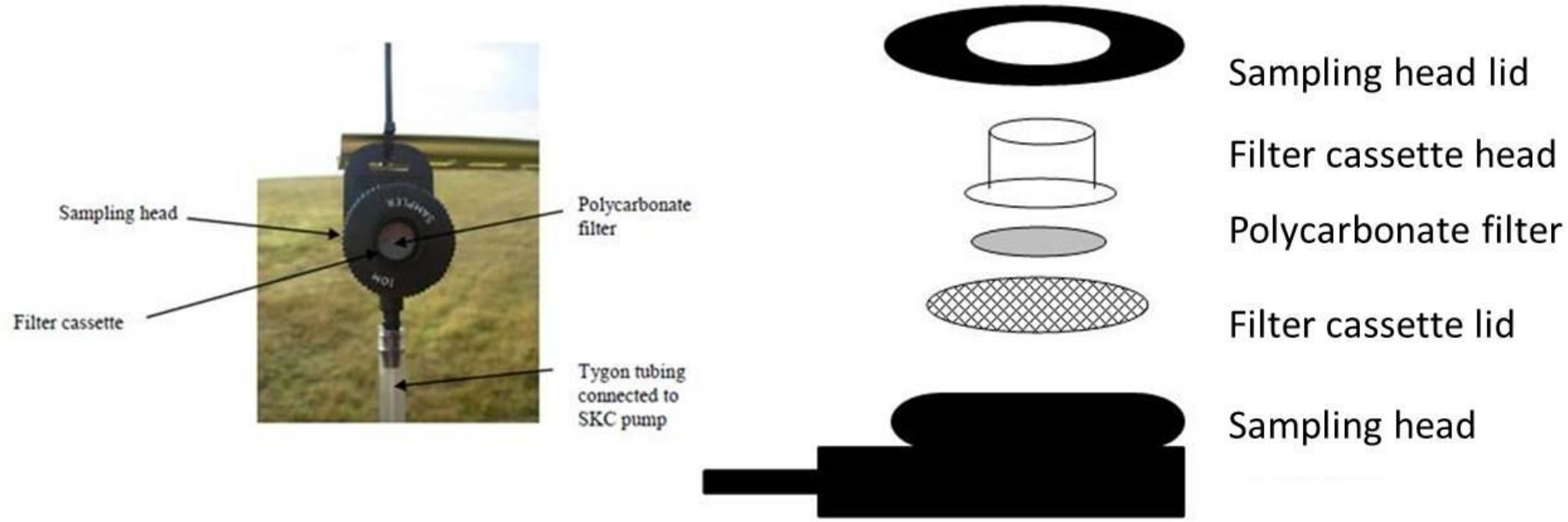

Figure 8-9 Illustration of the sampling equipment. Left: The sampling equipment as it appears when in use, taken from Pankhurst *et al.*, (2010). Right: The components of the sampling head

SKC personal samplers were mounted on long, sturdy, lengths of metal, as illustrated in Figure 8-10. This allowed the sampling heads to be placed as close as physically possible to the agitation activities, without posing harm to the sampler. To ensure the safety of the sampler, all experimental work was carried out at Amey Cespa on a Sunday, when the site is normally closed. A single site operator carried out agitation activities under the management of the sampling team. This was advantageous because:

- It ensured maximum safety of the samplers, whereby vehicle movements were pre-planned
- The samples were representative of a single agitation activity – if working within normal operational hours, several agitation activities may occur at once, potentially contaminating any samples

Turning, screening and shredding agitation activities were sampled as described in section 8.6.1. Each agitation activity was sampled three times in a single visit.

Immediately after sampling, the cassettes containing the filters were removed and wrapped in clean foil to avoid further contamination and allow transportation back to the laboratory. All filters were transported to and from the sampling site in a cool box at a temperature of approximately 4ºC.

A photograph of the novel sampling equipment in use is presented in Figure 8-11.

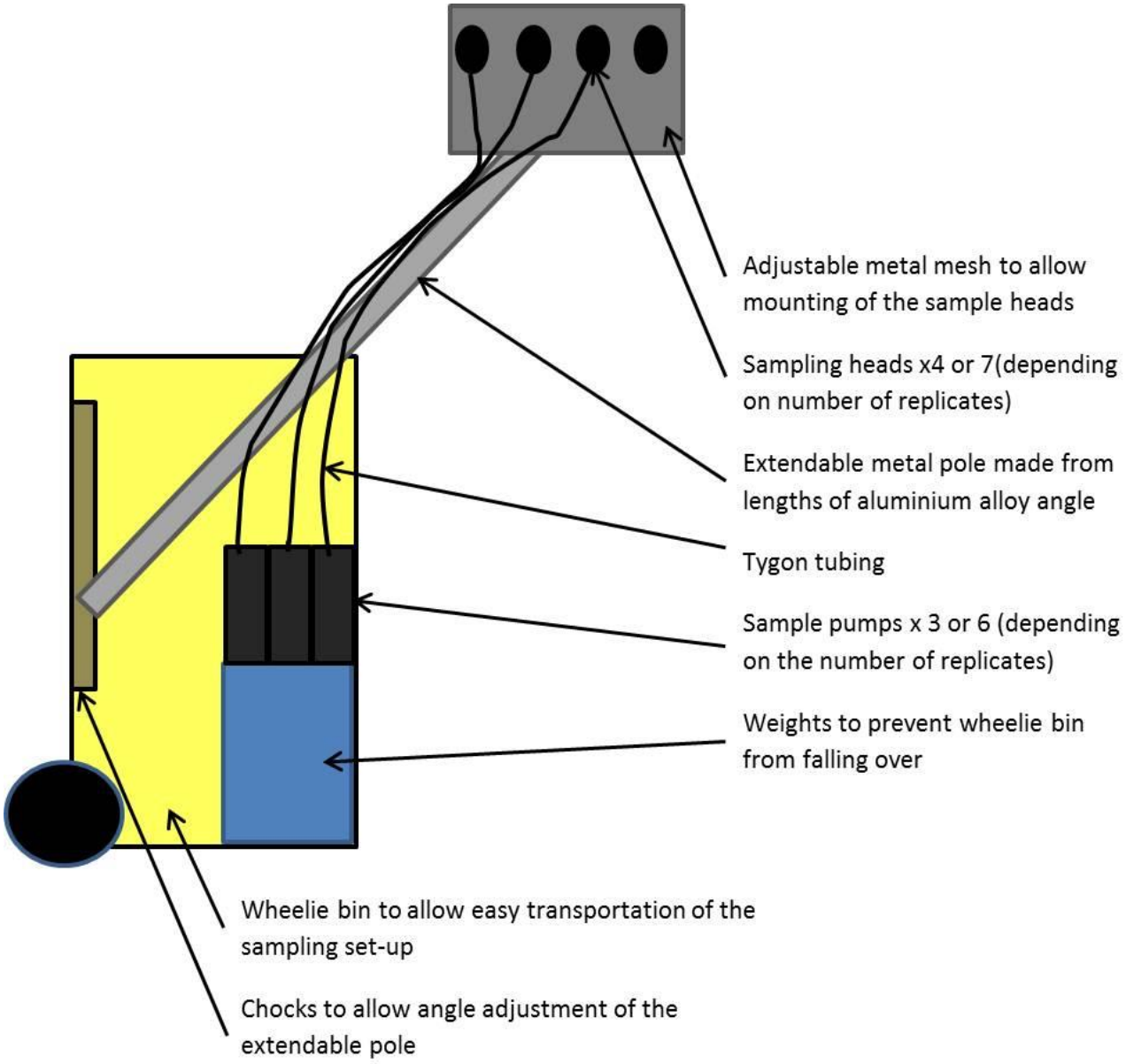

Figure 8-10 Illustration of the equipment used to allow bioaerosol sample collection <30cm from agitation activities

Figure 8-11 A photograph of the sampling equipment illustrated in Figure 8-10 in-use during turning activities at Amey Cespa. The highlighted area is a front end loader agitating the compost, demonstrating the proximity of the sampling equipment to the agitation activities. The arrows point out the rods used to estimate pollutant exit velocity as discussed in section 8.5.1

8.6.2.3 Post-sampling processing

Samples were processed within 24 hours of collection to prevent loss of viability. All work was carried out aseptically, following the methods stated in the standard protocol (AfOR, 2009) which is outlined below:

- Filters were removed from cassettes with flame sterilised tweezers. The filter was placed into 5 millilitres of sterile buffer solution and shaken for 15 minutes at 35ºC.
- A serial dilution was made whereby 1 millilitre of the suspension was transferred to 9ml of saline solution. Immediately before dilution, the suspension was shaken for 1 minute
- 100 microliters of each sample were inoculated in triplicate onto the pre-prepared media plates under aseptic conditions. The inoculum was spread evenly over the surface of the agar using aseptic L-shaped spreaders

The samples were then incubated as per the standardised protocol, (AfOR, 2009). NA and MAC were incubated at 37ºC for 2-7 days. MEA was incubated at 40ºC for 2-3 days. Plates were checked for growth daily, and were counted as soon as growth was visible. When counting colonies, the colour and shape of the colonies were also recorded.

8.6.2.4 Quality control

Aseptic techniques were adopted wherever necessary. Equipment was sterilised in an autoclave at 121ºC for 15 minutes, all surfaces were wiped regularly with 70% ethanol, and all equipment was handled within a class 2 laminar flow cupboard and within 30cm of a Bunsen burner. To check whether sterility was achieved, agar plates inoculated with sterile buffer solution were incubated. Agar plates without an inoculum were also incubated. To check whether the selective media was working, positive controls were taken. NA was inoculated with an existing culture of *Staphylococcus aureus,* a Gram-positive Bacterium, MAC with *Escherichia coli,* a Gram-negative Bacterium, and MEA with *Aspergillus fumigatus,* a fungus.

On-site, two blanks per sampling location were retained and enumerated. A blank is treated in the same way as a regular sample, but without the use of a pump (AfOR, 2009). Firstly, a handling blank was taken whereby a sterile filter was placed into a sampling head and then immediately removed, to identify possible contamination when handling the filters. Secondly a blank was taken by placing a sterile filter into a sampling head disconnected from a pump, and exposing it to the air for the same period of time as the rest of the samples. This determines the number of bioaerosols that impacted the filter naturally without the aid of a pump.

8.6.2.5 Enumeration

To calculate the concentration of bioaerosols present in the air at the time of sampling, Equation 8-2 was used:

$$C = \frac{(n/I)V}{(FD)/1000}$$

Equation 8-2

Where:

C is the bioaerosol concentration in air (CFU/m^3)

n is the average number of colonies retained acroos replicates. If plate growth was overcrowded then values from the next dilution were used, and multiplied up accordingly

I is the volume of inoculum plated (ml). This was equal to 0.1 throughout the project

V is the volume of buffer solution in the original vial (ml). This was equal to 5 throughout this project

F is the sampling flow rate (L/min). This was equal to 2 throughout the project

D Is the sampling duration (minutes). This was equal to 2 through the project

As samples were replicated on-site and in the laboratory, mean averages of the concentrations calculated for each replicate were reported and used throughout the statistical analysis.

A lower limit of detection [LLOD] as described in Pankhurst (2010) can be calculated by assuming the growth of one colony averaged across all replicates.A mean average number of colonies retained (n in Equation 8-2) can be calculated by applying this assumption, and Equation 8-2 can be utilised to calculate the LLOD. The LLOD in this project varies depending on the number of replicates taken and the sampling duration used. Field replicates were taken in triplicate or sextuplet, and a sampling duration of 2 minutes was used, as described in section 8.6.2.2. Three laboratory replicates were consistently produced. This information was inputted into Equation 8-2 and resulted in a

LLOD for each sampling condition. A worked example for calculating the LLOD when sampling in triplicate for 2 minutes, is provided below:

$$\frac{(0.111/0.1)x5}{(2x2)/1000} = 1388 \text{ CFU/m}^3$$

The LLODs for each of the conditions used in this project areprovided in Table 8-6.

Table 8-6 LLODs for each of the sampling conditions used in the project

Number of field replicates	Sampling time (minutes)	Resultant LLOD (CFU/m^3)
3	2	1388
6	2	695

Any potential bioaerosol levels found in lower concentrations than those reported in Table 8-6 will not be detected using the sampling methods employed in this study. Therefore any apparent 'zero' values may be equal to any concentration between 0 and the LLOD minus 1. Therefore any zero values are presented as '<LLOD'.

8.6.2.6 Statistical analysis

The statistical analysis methods are identical to Pankhurst (2010) and thus are outlined briefly. Data were statistically analysed using a General Linear Model [GLM] in Statistica version 10 (Statsoft®, 2012). A GLM incorporates a series of statistical tests, including ANOVA, MANOVA, ANCOVA, and multiple linear regression, into one simple process (StatSoft, 2012). This allows the analysis of within effects in the data. A within effect is when the same test is administered to a set of data measured repeatedly over time, or under other different circumstances (StatSoft, 2012).

The results of a GLM are reliable only when the input data has a normal distribution. Data normality can be checked by producing a normal probability plot of the raw residuals. When completing this step it was apparent that the data was not normally distributed, and therefore a natural log transformation of

the raw data was made. To allow the log transformation, zero values within the data were altered. Zero values were altered to one lower than the LLOD to represent a 'worst case scenario'. Residuals of the transformed data were checked, confirming that the data transformation was successful, and the data was normally distributed.

A Fisher Least Significant Difference [LSD] test was used to identify statistical differences or similarities between sampling visits, locations and bioaerosol types. A Fisher LSD is a post-hoc test that determines if there are any significant differences between group means (Statistica, 2012). Any significant similarities can be identified and used to annotate graphical representations of the data. This allows easy identification of results that are statistically similar or different. This is explained in more detail in Pankhurst (2010). Table 8-7 illustrates how the Fisher LSD test provides the annotations and Figure 8-12 demonstrates how the annotations are applied.

Table 8-7 An example of how statistical similarities and differences are determined via a Fisher LSD test. An 'x' identifies that the specified annotation label should be used for a particular sampling location in graphical representations of the data

Sampling location	Mean of the natural log transformed sampled data	Annotation labels	
		a	b
1	13.34	X	
2	8.24		X
3	11.45	X	X
4	13.16	X	

Sampling locations with identical annotation labels, as identified in the example illustrated in Table 8-7, are statistically identical. In the example illustrated in Table 8-7, the data for locations 1 and 4 have identical annotation labels and therefore the data are statistically the same. The data for sampling location 3 does have the same annotation label as the data for locations 1 and 4, but with the addition of a further annotation label. This indicates that the data for location

3 are statistically similar, but not identical, to the data for locations 1 and 4. The data for sampling location 2 has a different annotation label than the data for locations 1 and 4. This indicates that the data are statistically different. However, the data for location 2 does share an annotation label with the data for sampling location 3, indicatingthat the data for locations 2 and 3 are statistically similar. These annotations are applied graphically in Figure 8-12.

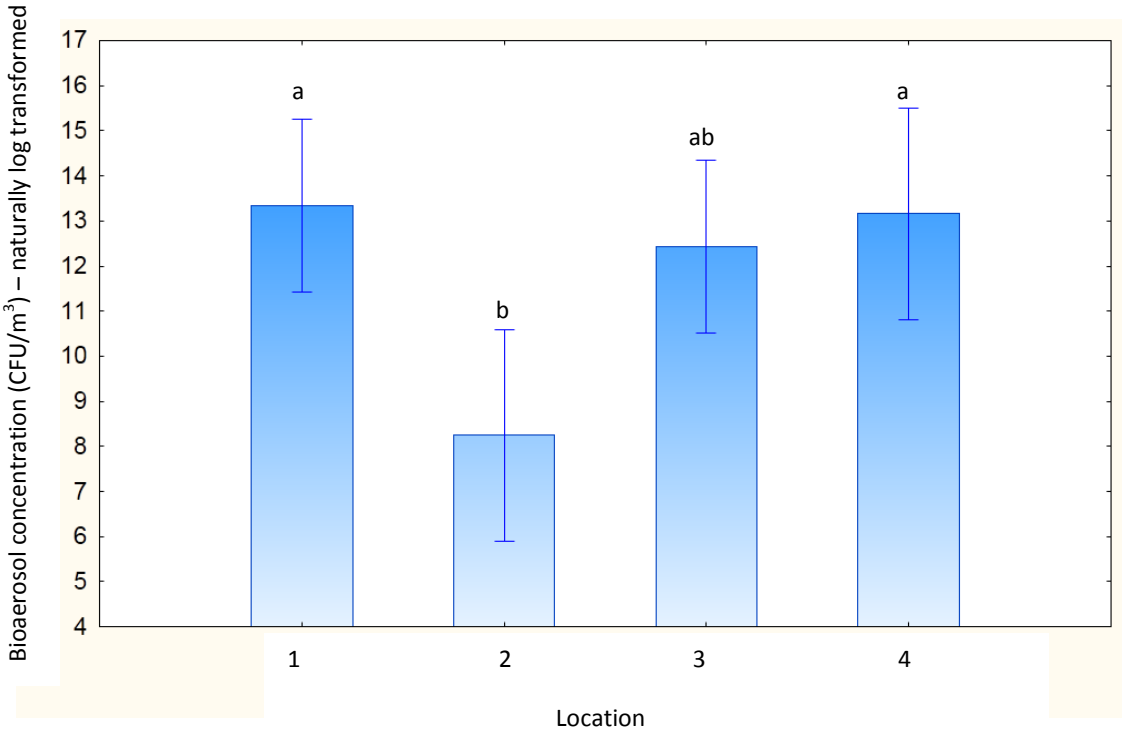

Figure 8-12 Graphical application of Fisher LSD annotations to example data. Bars represent the mean average of the sampled data. The error bars denote 0.95 confidence intervals

Figure 8-12 shows that the statistical similarities and differences within the data can be clearly identified using the annotations provided when completing a Fisher LSD test.

8.6.3 Results

Bioaerosol concentrations obtained using the sampling techniques described above, during agitation activities, are presented in Table 8-8. Due to site operations during the autumn visit, shredding activities were sampled indoors. It was not possible to sample shredding activities during the spring visit, due to a mechanical failure with the shredding machine.

Table 8-8 Bioaerosol concentrations obtained when sampling within 30cm of composting agitation activities. The values presented have been averaged across the field and laboratory replicates. '*' indicates that the activity was performed indoors. All values presented have been rounded to 2 decimal places

Bioaerosol	Season	Activity	Minimum concentration (CFU/m^3)	Maximum concentration (CFU/m^3)	Mean Average concentration (CFU/m^3)
Aspergillus fumigatus	Autumn	Turning removal	$<6.95x10^2$	$4.03x10^4$	$1.62x10^4$
		Turning Deposit	$<6.95x10^2$	$4.17x10^3$	$2.55x10^3$
		Screening	$1.94x10^4$	$3.72x10^4$	$2.86x10^4$
		Shredding*	$<1.39x10^3$	$3.15x10^5$	$1.19x10^5$
	Winter	Turning removal	$3.42x10^4$	$8.10x10^5$	$3.15x10^5$
		Turning Deposit	$1.25x10^5$	$1.97x10^6$	$7.62x10^5$
		Screening	$9.58x10^3$	$1.13x10^6$	$3.87x10^5$
		Shredding	$1.54x10^5$	$2.06x10^5$	$1.78x10^5$
	Spring	Turning removal	$2.78x10^3$	$2.92x10^5$	$1.23x10^5$
		Turning Deposit	$4.17x10^3$	$6.51x10^5$	$2.23x10^5$
		Screening	$<6.95x10^2$	$4.31x10^4$	$1.52x10^4$
Total Bacteria	Autumn	Turning removal	$4.82x10^5$	$8.36x10^5$	$6.73x10^5$
		Turning Deposit	$3.09x10^5$	$1.01x10^6$	$6.26x10^5$
		Screening	$4.29x10^5$	$1.59x10^6$	$1.08x10^6$
		Shredding*	$<1.39x10^3$	$3.15x10^5$	$1.98x10^5$

Bioaerosol	Season	Activity	Minimum concentration (CFU/m^3)	Maximum concentration (CFU/m^3)	Mean Average concentration (CFU/m^3)
Total Bacteria	Winter	Turning removal	$1.96x10^5$	$6.85x10^5$	$3.69x10^5$
		Turning Deposit	$3.13x10^4$	$2.23x10^6$	$7.89x10^5$
		Screening	$6.08x10^4$	$1.01x10^6$	$5.75x10^5$
		Shredding	$6.25x10^4$	$1.42x10^5$	$1.07x10^5$
	Spring	Turning removal	$1.28x10^6$	$3.18x10^6$	$2.48x10^6$
		Turning Deposit	$1.04x10^6$	$4.06x10^6$	$2.65x10^6$
		Screening	$2.04x10^6$	$3.49x10^6$	$2.69x10^6$
Gram-negative Bacteria	Autumn	Turning removal	$9.03x10^3$	$6.25x10^4$	$3.13x10^4$
		Turning Deposit	$<6.95x10^2$	$4.51x10^4$	$2.43x10^4$
		Screening	$1.67x10^4$	$2.71x10^5$	$1.26x10^5$
		Shredding*	$<1.39x10^3$	$1.53x10^4$	$5.09x10^3$
	Winter	Turning removal	$8.82x10^4$	$2.08x10^5$	$1.34x10^5$
		Turning Deposit	$1.32x10^4$	$4.82x10^5$	$2.18x10^5$
		Screening	$2.04x10^5$	$7.11x10^5$	$3.79x10^5$
		Shredding	$4.03x10^4$	$3.88x10^5$	$2.30x10^5$
	Spring	Turning removal	$1.56x10^5$	$5.92x10^5$	$3.72x10^5$
		Turning Deposit	$5.65x10^5$	$8.33x10^5$	$6.71x10^5$
		Screening	$2.47x10^5$	$4.43x10^5$	$3.23x10^5$

Table 8-8 shows that the concentration of bioaerosols collected close to the agitation activities varies, covering several orders of magnitude from below the LLOD to 4.06x10^6 CFU/m3. To interpret this data more comprehensively, the data in Table 8-8 was statistically analysed as described in section 8.6.2.6. The statistically analysed results for *Aspergillus fumigatus,* Total Bacteria and Gram-negative Bacteria are presented in Figure 8-13, Figure 8-14, and Figure 8-15 respectively.

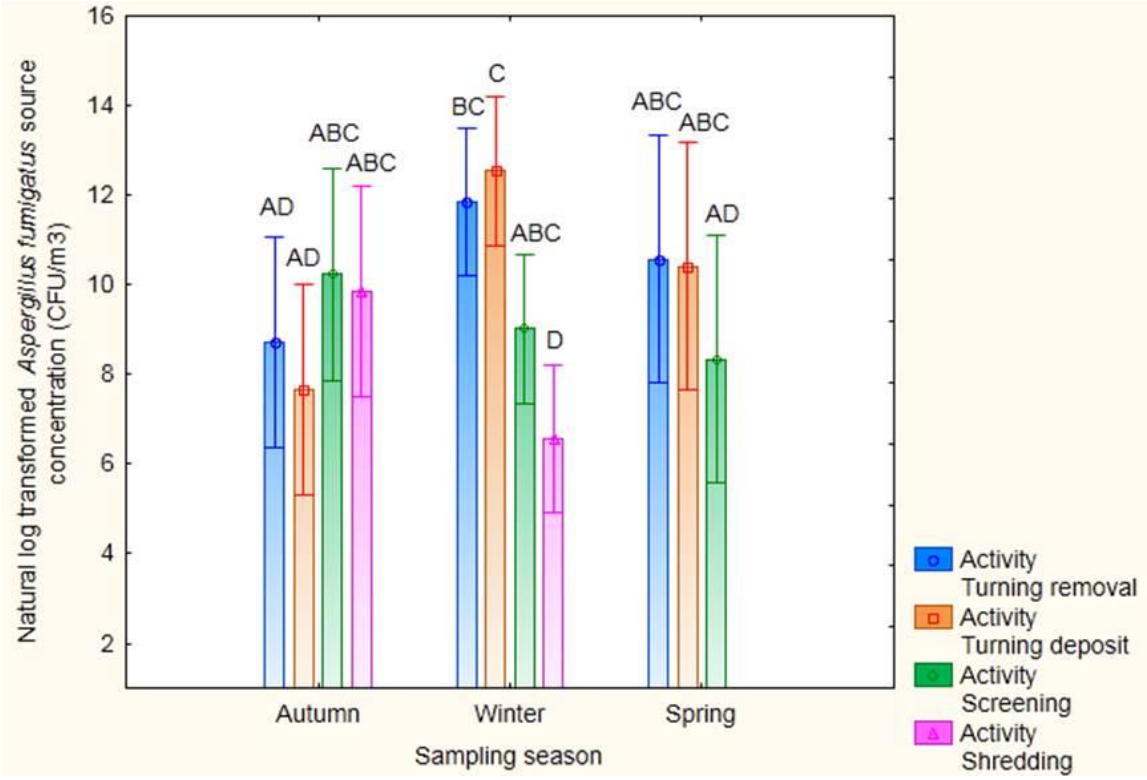

Figure 8-13 Mean average *Aspergillus fumigatus* source concentration results. Please note that the graph displays natural log transformed concentration data. Error bars represent a 0.95 confidence interval. The letters above the bars are statistical annotations, denoting values of statistical similarity

Figure 8-13 shows thatthe turning removal and turning depositing activities are statistically identical for the spring sampling, and are statistically similar for autumn and winter sampling. It also appears that the highest turning concentrations were captured during the winter. Considerable ower concentrations of *Aspergillus fumigatus* were captured during shredding activities in the winter and summer, but not in the autumn,

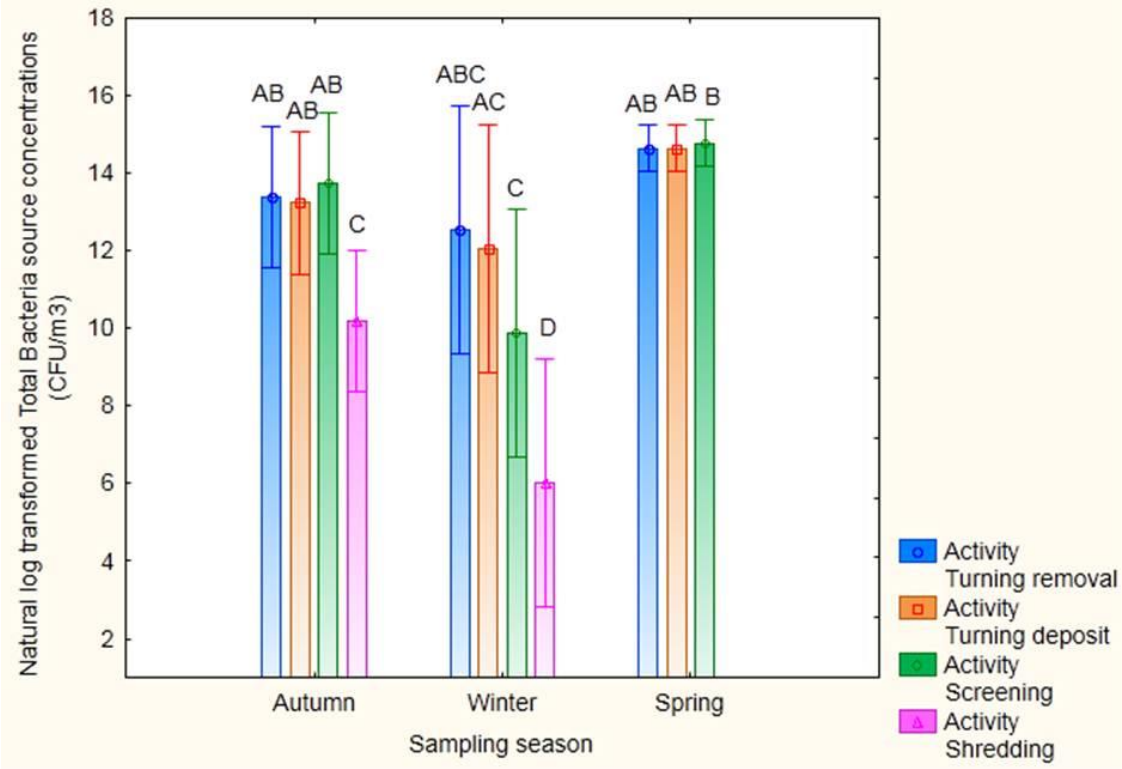

Figure 8-14 Mean average Total Bacteria source concentration results. Please note that the graph displays natural log transformed concentration data. Error bars represent a 0.95 confidence interval. The letters above the bars are statistical annotations, denoting values of statistical similarity

It can be seen in Figure 8-14 that the agitation activities sampled in spring and and autumn are statistically similar. For winter and autumn samples, the shredding activity is statistically different to the other agitation activities, having much lower Total Bacteria source concentrations. In winter, the concentrations of Total Bacteria during screening activities are also lower than those observed during autumn and spring.

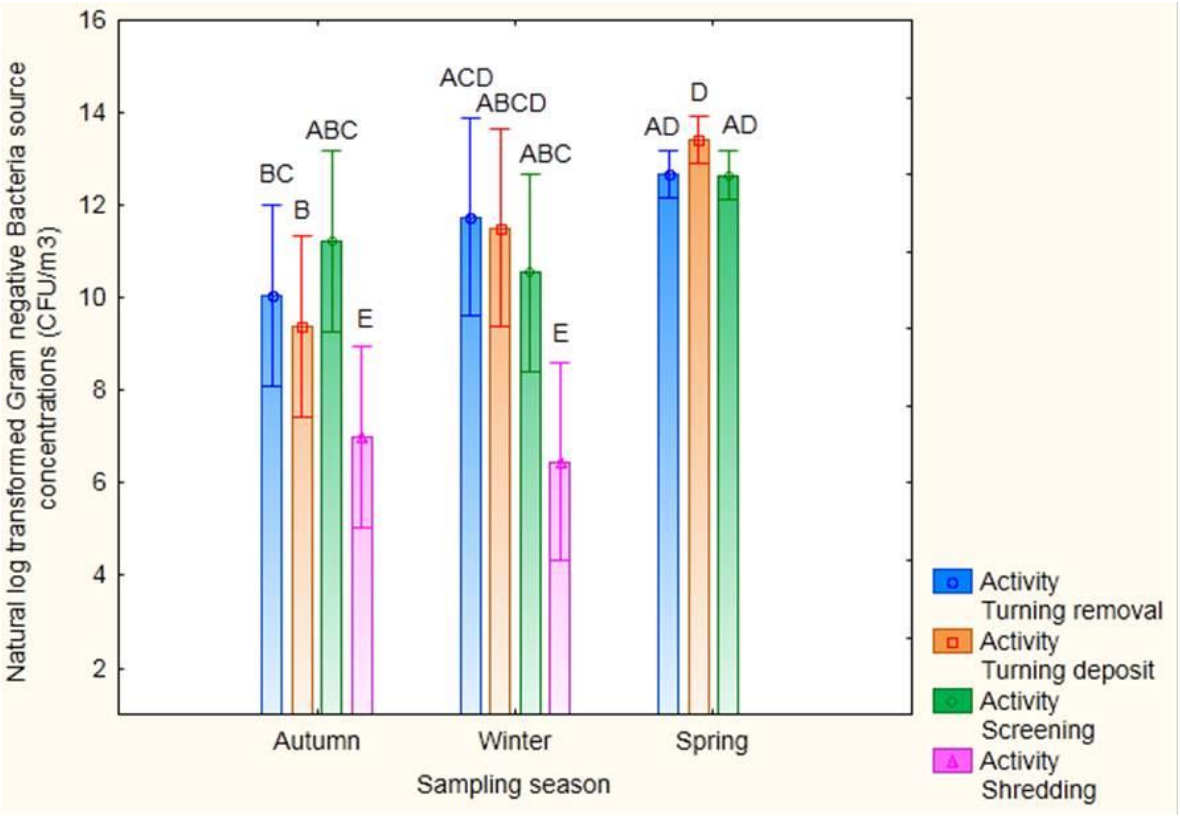

Figure 8-15 Mean average Gram negative Bacteria source concentration results. Please note that the graph displays natural log transformed concentration data. Error bars represent a 0.95 confidence interval. The letters above the bars are statistical annotations, denoting values of statistical similarity

Figure 8-15 shows that in autumn and winter the measured bioaerosol concentrations during shredding activities are consistently lower than the turning and screening activities. During all seasons, the turning and screening activities are statistically similar.

Observing the results across all seasons and for each bioaerosol type in Figure 8-13, Figure 8-14 and Figure 8-15 overall it can be considered that:

- The turning removal, turning deposition and screening activities are mostly statistically similar
- In the majority of cases, the shredding activity is statistically different to all the other activities, providing lower source concentration values
- Generally Total Bacteria concentrations were the highest, followed by Gram-negative Bacteria and *Aspergillus fumigatus* concentrations

8.7 Pollutant emission rate calculations

Quantification improvements have now been completed to provide improved bioaerosol concentration and exit velocity values at the source of the agitation activities.. These values, along with knowledge of the agitation geometry (as estimated by observations detailed in section 8.6.1 and section 8.7.2 below, and using agitation machinery technical specifications) can now be used to calculate a pollutant emission rate.

8.7.1 Equations

After consulting with the ADMS model developers, CERC (Strickland, 2011), the equation used by Taha *et al.,* (2005; 2006; 2007) and Drew *et al.,* (2007) to calculate fugitive bioaerosol emissions in a wind tunnel adapted from Jiang and Kaye (2001), was modified to calculate bioaerosol emission rates from agitation activities. Equation 8-3 was used to calculate a bioaerosol emission rate assuming a point source.

$$E = FB$$ **Equation 8-3**

Where: E is the emission rate (CFU/s)
F is the volume flow rate (m^3/s) calculated using Equation 8-4
B is the bioaerosol concentration at the source of the agitation activity (CFU/m^3), as measured in section 8.6

The flow rate was calculated using Equation 8-4.

$$F = RV$$ **Equation 8-4**

Where: R is the area of the pollutant release (m^2) calculated using Equation 8-5
V is the velocity of the release (m/s), as estimated in section 8.5

The area of the pollutant release was calculated using Equation 8-5.

$$A = \pi r^2$$ **Equation 8-5**

Where r is the radius of the point source in metres.

$$A = LW$$ **Equation 8-6**

Where: L is the length of the source

W is the width of the source

Equation 8-3 can also be adapted to calculate bioaerosol emission rates from line, area and volume sources (Strickland, 2011), by dividing by the dimensions of the source, in m, m^2 and m^3 for line, area and volume sources respectively, altering the units of the emission rate to CFU/m/s, CFU/m^2/s and CFU/m^3/s correspondingly.

8.7.2 Source representation

Traditionally point sources have been used to represent bioaerosol emissions from agitation activities (Millner *et al.,* 1980; Danneberg *et al.,* 1997; Taha *et al.,* 2006;2007; Drew *et al.,* 2007; SNIFFER; 2007). However, the model was calibrated and validated (Chapters 5, 6 and 7) with some success by modelling bioaerosol emissions as an area source. Several area sizes were tested, and an area size representing the size of a compost windrow provided the best correspondence between the modelled and measured data. The observations described in section 8.6.1, revealed the complexity of the agitation activities, detailing that an agitation activity can be comprised of several components. Therefore it may not be appropriate to represent the source in a simplistic manner, and more suitable to represent an agitation activity as a series of bioaerosol emissions of varying size and strength. As discussed in section 2.5.2, several source types are available in ADMS, designed to represent different scenarios. Multiple source types and combinations are possible in the ADMS model. Initiation of emissions over varying time periods is also achievable in the ADMS model, allowing the modeller to simulate emissions as simply or complexly as required. Summarising the source types available in the ADMS model:

- Point sources are circular, and are specified by diameter, height, and the coordinates of their centre (CERC, 2010b). Point sources are normally used to represent pollutant stacks (SNIFFER, 2007) where the dimensions of the stack are well defined and easy to measure
- Jet sources are releases where the pollutant exit velocity has vertical and horizontal components. Like point sources, they are specified by diameter, height, and coordinates of the centre as well as angle of the release (CERC, 2010b)
- A line source is a uniform release along a straight line at the same source height. The line is specified by width, height, and coordinates of the centre points of its extremities (CERC, 2010b)
- An area source has three or more vertices, and is specified by width, length, height and coordinates of the vertices (CERC 2010b). Thus an area source is a release over a horizontal plane at a specified height, and the emission is assumed to be uniform across the area (CERC, 2010b)
- Volume sources, similarly to area sources, have three or more vertices, and are specified by width, length, depth and coordinates of the vertices (CERC, 2010b). Volume sources are often used to represent fugitive emissions from buildings (CERC, 2010b).

At present there is not enough knowledge on bioaerosol emissions to suggest that releases have both vertical and horizontal components, therefore jet sources will not be considered in this study. As volume sources are typically used to represent emissions from buildings, and this study focusses on outdoor windrow composting, volume sources will also not be considered at this stage.

Considering the agitation actions as detailed in section 8.6.1, line, point and area sources may all be appropriate to represent different components of the agitation activities. Turning actions 1 and 3 and consequently shredding actions 1, 3, 5 and 7, and screening actions 1, 3, 5, 7, 9, and 11 could be considered to be small point or area sources. Additionally an area source provided the best fit between the modelled and measured data in Chapters 5 and 6, whereas point

sources have been traditionally used to represent agitation activities in previous studies (Millner *et al.,* 1980; Danneberg *et al.,* 1997; Taha and Pollard, 2004; Taha *et al.,* 2006; 2007; Drew *et al.,* 2007; SNIFFER, 2007; Tamer Vestlund, 2009). Therefore emission rates were calculated for both point and area sources based on the observations made in this study.

Turning action 2, and thus shredding actions 2 and 6 and screening actions 2, 6 and 10 could be considered as line source, but emissions from these actions were considered to be negligible, and thus an emission rate was not calculated. Shredding action 4 and screening actions 4 and 8 could be considered to be more 'controlled' than turning agitation activities, as they are performed on machinery situated in a fixed place. The emissions are also constrained somewhat to the dimensions of the apparatus. As neither the screening nor shredding machinery is circular, a point source was not considered for these agitation activities (Doppstadt, 2009a; 2009b). It was only possible to sample emissions from at a single location during the screening and shredding activities, therefore a small area source will be used to represent the approximate area of the emission sampled.

A summary of the source dimensions used in the emission rate calculations, with explanations of how these dimensions were estimated is provided in Table 8-9.

Table 8-9 Source dimensions for each source type and agitation activity, with explanations, used to calculate emission rate

Agitation activity	Source type	Dimension used (m)	Explanation
Turning removal and Turning deposit	Point	3	Simplified version of the turning area source type, as described below
	Area	3x2	Bioaerosol measurements were taken immediately above the agitation activity. From observations, an area slightly larger than the bucket of the FEL was agitated, as material around the void, created by the FEL bucket, collapsed into the cavity during turning removal. Similarly, an area slightly larger than the bucket was disturbed when material was deposited from the FEL bucket. Therefore the dimensions used were slightly larger than the size of a typical FEL bucket (Volvo, 2009).
Screening	Area	2.5x2.5	Bioaerosol measurements were taken immediately above where the material exited the screening machine, as described in section 8.6.1.3. Therefore, the width of a typical screening machine was used to represent the dimensions of the emission area that was sampled (Doppstadt, 2009b)
Shredding	Area	2x2	Similarly to screening, bioaerosol measurements were taken immediately above where the material exited the shredding machine. The width of a typical shredding machine was used to represent the area of the emission that was sampled (Doppstadt, 2009a)

As shown in Table 8-9, a line source was not considered when calculating emission rates. A line source is used to represent emissions uniformly emitted along a straight line (CERC, 2010b). As the bioaerosol measurements were taken at a single location, for example immediately above a turning activity, or where material exited a machine, a line source type was not considered appropriate at this stage. However, if in the future emissions are measured in a

straight line at a uniform height above an agitation activity, then this source type could be considered.

8.7.3 Calculations

Pollutant exit velocities were estimated for the turning, screening and shredding agitation activities performed during the autumn season, and the screening agitation activity during the winter season, both completed at Amey Cespa, as described in section 8.5. Therefore it was only possible to calculate emission rates during these agitation activities, using Equation 8-3 (modified and unmodified), Equation 8-4 and if necessary, Equation 8-5 as described in section 8.7.1. The corresponding bioarosol concentrations, presented in Table 8-8 were used to calculate an emission rate during these agitation activities.

The dimensions of each source were estimated via observations and using technical specifications of the machinery used to agitate the compost (Doppstadt, 2009a; 2009b; Volvo, 2009) as described in Table 8-9. Emission rates for point and area source types were calculated for the turning removal, turning depositing, screening and shredding actions, as described in section 8.7.2.

The calculated emission rates are presented in Table 8-10, alongside the values used to calculate the emission rate. Table 8-10shows that the calculated emission rates cover several orders of magnitude. Emission rates calculated for point sources varied from 3.60×10^4 to 1.41×10^7 CFU/s and emission rates calculated for area sources varied from 1.53×10^3 to 2.16×10^6 CFU/m^2/s. Area source types resulted in lower calculated emission rates when compared to point sources.

It was not possible to perform any dispersion modelling using these calculated emission rates, or any of the improved parameters attained in this chapter. This is because it was not possible to collect bioaerosol concentration data downwind of the agitation activities, to allow a direct comparison to the modelled outputs, due to equipment and time constraints.

Table 8-10 A summary of the parameters and consequential estimated emission rates calculated based on the information gained from this study. The notations 'AF', 'TB', and 'GN; correspond to *Aspergillus fumigatus,* Total Bacteria and Gram-negative Bacteria respectively.

Agitation Activity	Season	Source type	Bioaerosol type	Bioaerosol concentration (CFU/m^3)	Source dimension (m)	Pollutant exit velocity (m/s)	Calculated emission rate (units)
Turning removal	Autumn	Point	AF TB GN	16204 672801 31250	3 (diameter)	3	$3.40x10^5$ (CFU/s) $1.41x10^7$ (CFU/s) $6.56x10^5$ (CFU/s)
Turning removal	Autumn	Area	AF TB GN	16204 672801 31250	3x2	3	$4.86x10^4$ ($CFU/m^2/s$) $2.02x10^6$ ($CFU/m^2/s$) $9.38x10^4$ ($CFU/m^2/s$)
Turning depositing	Autumn	Point	AF TB GN	2546 625810 24306	3 (diameter)	3	$3.60x10^4$ (CFU/s) $8.85x10^6$ (CFU/s) $1.62x10^6$ (CFU/s)
Turning depositing	Autumn	Area	AF TB GN	2546 625810 24306	3x2	3	$7.64x10^3$ ($CFU/m^2/s$) $1.88x10^6$ ($CFU/m^2/s$) $7.29x10^4$ ($CFU/m^2/s$)
Screening	Autumn	Area	AF TB GN	28588 1081134 126389	2.5x2.5	2	$5.72x10^4$ ($CFU/m^2/s$) $2.16x10^6$ ($CFU/m^2/s$) $2.53x10^5$ ($CFU/m^2/s$)

Agitation Activity	**Season**	**Source type**	**Bioaerosol type**	**Bioaerosol concentration (CFU/m^3)**	**Source dimension (m)**	**Pollutant exit velocity (m/s)**	**Calculated emission rate (units)**
Screening	Winter	Area	AF TB GN	386667 575139 378889	2.5x2.5	0.5	4.33x10^4 (CFU/m^2/s) 2.88x10^5 (CFU/m^2/s) 1.89x10^5 (CFU/m^2/s)
Shredding	Autumn	Area	AF TB GN	119444 198148 5093	2x2	0.3	3.58x10^4 (CFU/m^2/s) 5.94x10^4 (CFU/m^2/s) 1.53x10^3 (CFU/m^2/s)

8.8 Discussion

8.8.1 Discussion of the pollutant temperature results

Measured pollutant temperatures were found to be consistently above ambient temperature. This result was expected as the core of the composting core can reach in excess of 55°C (Lacey and Crook, 1988). The temperature of the whole visible pollutant plume was measured, and it was observed that the temperature of the plume decreased rapidly upon release. In the majority of the TIs analysed, plume rise was apparent. These findings correspond to the conceptual pollutant temperature perceptions illustrated in Figure 2-4.

The highest measured pollutant temperatures originated from turning activities. As turning activities are performed on windrows that have remained static for prolonged periods of time, the temperature of the core of the compost increases, as previously described in section 2.2.3. The 'main phase' in which turning activities are completed within is also the most biologically active phase of the composting process (Swan *et al.,* 2003). Therefore it was expected that high temperatures would result from this agitation type. As highlighted in section 8.6.1, the shredding and screening activities are comprised of many components, including transportation of the composting material into the machinery. Therefore the compost has been exposed to the ambient air for an extended time prior to entering the shredding or screening machinery, allowing the compost to cool, and thus yielding lower pollutant temperatures than turning activities. It was also observed that the emissions from the turning activities were more sporadic than compared to the shredding and screening activities. This again was expected as the turning actions are not continuous, as the FELs used to complete the activity are constantly transferring compost to various locations to enable the completion of the turning activity, as described in section 8.6.1.1. Screening and shredding activities are more continuous as the machinery is constantly in motion, but in a fixed location.

The range of pollutant plume temperatures acquired from this study was 3.7 – 29.5°C collected in varying ambient temperatures. This corresponds well to the

pollutant temperatures used in previous modelling studies reported in the literature which varied from 9.5 to 30°C (Taha and Pollard, 2004; Drew *et al.,* 2005; 2007; Taha *et al.,* 2006; 2007). However, it is not known how the majority of the pollutant temperatures published in the literature were measured or estimated. Therefore it is not possible to suggest why or how the pollutant temperatures measured in this study correspond to those previously published. The results presented in this chapter are the first known attempts to measure the pollutant plume temperature of bioaerosols emitted from open windrow composting facilities.

8.8.2 Discussion of the pollutant exit velocity results

It was anticipated that the ambient wind speed would affect the results. The pollutant exit velocity was predicted by observing plume movements outdoors. Therefore as the pollutant exit velocity was not measured at the instant point of release, it was assumed that the pollutant plume movement was effected by the ambient wind speed. Open windrow composting processes are mostly performed outdoors, and thus emissions are subjected to local meteorological conditions. Therefore it was expected that an increase in ambient wind speed would result in an increase in the perceived pollutant exit velocity. This was observed in the results, as when the ambient wind speed decreased, so did the estimated pollutant exit velocity. However, due to site operations on the day of sampling, observations of pollutant exit velocity during shredding activities were performed indoors. Indoor activities are not subject to the same ambient conditions as those performed outside, and thus may represent a more accurate estimation of the pollutant exit velocity.

It was apparent that the turning activities resulted in generally higher estimated pollutant exit velocities. Similarly to observations of pollutant temperature, a rapid pollutant plume rise was expected during turning, as the hotter core of the compost is exposed to cooler ambient temperatures. As shredding and screening activities are performed on material that has been exposed to ambient air for prolonged periods of time, less plume rise and thus lower pollutant exit velocities were expected, and this was observed in the results.

Exit velocities of 0.19 m/s (Drew *et al.,* 2005) and 0.20 m/s (Taha *et al.,* 2007) have been reported. The exit velocities estimated in this study range from 0.3 to 3.0 m/s, which are consistently higher than the values reported in the literature. However, as it is not apparent how the values reported in the literature were measured or estimated and thus it is not possible to speculate why this difference in values was observed. The results detailed in this chapter are the first known justified estimates of pollutant exit velocity of bioaerosol emissions from open windrow composting facilities. However the methods that were used to estimate the pollutant exit velocity were very basic, and limited, as discussed in more detail in section 8.8.5.

8.8.3 Discussion of the results of the bioaerosol concentrations collected at source

Bioaerosol concentrations were measured during two components of the turning activity; material removal and material deposition, based on observations of the site activities. Results indicated that statistically there was no significant difference between these turning agitation components. Shredding activities generallyresulted in lower bioaerosol concentrations when compared to the turning and screening agitation activities. This was unsurprising as periods of high rate biological activity are not observed until the main phase of composting (Swan *et al.,* 2003). There was no apparent seasonal variation between the bioaerosol concentrations sampled during the different agitation activities. However, one set of emission measurements from only three seasons was captured. Neilsen *et al.* (1997), Recer *et al.* (2001) and Schlosser *et al.* (2009) all reported higher concentrations of bioaerosols during the summer and autumn months, contradicting the findings from this study. As discussed in Pankhurst (2010), the relationship between bioaerosol concentrations and season is not well understood, and seasonal trends may be influenced by site operational activities and practises.

Therefore it is recommended that further bioaerosol concentration measurements are performed during varying weather conditions.

Many bioaerosol concentrations measured during different composting agitation activities have been reported. Bioaerosol concentrations have been measured during different agitation activities (Weber *et al.,* 1993; Epstein, 1994; Pankhurst *et al.,* 2009; 2011) including turning (Lacey, 1997; Environment Agency, 2001b *et al.,* 2001; Sanchez-Monedero and Stentiford, 2003; Taha *et al.,* 2006; 2007; HSE, 2012) shredding, (Lacey, 1997; Environment Agency, 2001b; Sanchez-Monedero and Stentiford, 2003; SNIFFER, 2007; Taha *et al.,* 2007; HSE, 2010) and screening (Danneberg *et al.,* 1997; Environment Agency*,* 2001b; Sanchez-Monedero and Stentiford, 2003; Taha *et al.,* 2006; 2007; SNIFFER, 2007; HSE, 2010). Generally, when comparing the results from this study to bioaerosol concentrations from previous studies that have used the same sampling equipment and have sampled during similar agitation activities, the bioaerosol concentrations measured in this study were higher, by up to five orders of magnitude (Epstein, 1994). This is not surprising given the proximity of the sampling equipment to the agitation activities in this study, which was less than 0.3 metres from the source. In other studies bioaerosol concentrations were sampled at distances of 2 or more metres downwind of the source of the agitation activity. Concentrations sampled at these locations were expected to be lower to those collected in this study due to the rapid dispersal of pollutants upon release (Beychok, 1994).

8.8.4 Discussion of the results from the emission rate calculations

The bioaerosol emission rates calculated in this study ranged from $3.60x10^4$ to $1.41x10^7$ CFU/s for a point source and $1.53x10^3$ to $2.16x10^6$ CFU/m^2/s for an area source. These calculated rates correspond to previous emission rates: $2.0x10^1$ CFU/s (SNIFFER, 2007) to $6.7x10^{10}$ particles per second (Millner *et al.,* 1980) for point sources and $9.4x10^1$ (SNIFFER, 2007) to $5.3x10^6$ (Dowd *et al.,*2000) CFU/m^2/s for an area source, as detailed in Table 2-6. Observing the calculated emission rates presented in Table 8-10, the emission rates extend over three orders of magnitude. This is a much smaller range than the emission rates for agitation activities calculated via back extrapolation methods, which extend up to 16 orders of magnitude (Millner *et al.,* 1980; Danneberg *et al.,*

1997; Taha and Pollard 2004; ADAS, 2005; Taha *et al.,* 2006; Drew *et al.,* 2007; SNIFFER, 2007; Taha *et al.,* 2007). However the emissions calculated in this study were based on measurements from sampling events collected from a single composting site, and thus less variability was anticipated. The emission rates calculated for point sources were consistently higher than the emission rates calculated for area sources. This was expected, because when adapting Equation 8-3 to calculate emission rates from an area source, the equation is divided by the dimensions of that area, as described in section 8.7.1.

To calculate an emission rate, measurements of the pollutant exit velocity, dimensions of the source and bioaerosol concentrations at source were required. The measurements made to improve the quantification of these parameters were completed in this chapter. However, these measurements were subjected to many limitations, as discussed in section 8.8.5. As these parameters were utilised to calculate emission rates, the limitations associated with these measurements now impact upon the accuracy of the emission rate calculations. Overall, the main limitation of this emission rate estimation technique is the increased time and expense required to calculate an emission rate compared to methods such as back extrapolation. Emission rate estimations from back extrapolation can be completed in very short time scales, and inexpensively, whereas the method established in this study requires additional sampling and therefore time. Additionally, from the results of the model validation (Chapters 6 and 7) it is unclear whether site specific emission rates are required from site to site or not, and requires further investigation.

8.8.5 Limitations

8.8.5.1 Overall Limitations

The principal assumption made in this study is that the visible plume emitted from the agitation activities contains the highest concentrations of bioaerosols. As bioaerosols are not visible to the naked eye, it is not straightforward to view their travel and dispersion in the natural environment. However, it should be recognised that sensors, such as WIBS (Wide Issue Bioaerosol Sensor), are being developed to monitor the real-time continuous monitoring of bioaerosols

via biological fluorescence sensing (Kaye *et al.,* 2004; Foot *et al.,* 2008). Additionally, there is no evidence to suggest that bioaerosols would not be present in the visible plume, as it is well documented that some bioaerosol components can survive in thermophilic temperatures (Swan *et al.,* 2003).

The process of sampling on site was often difficult, due to health and safety implications. However samples were always taken as close to the source of the agitation activities as physical and safely possible. Where possible, measurements were completed remotely. For example using equipment such as the TIC, which did not require placement in the immediate vicinity of the activity.. The high health and safety risk factors associated with performing the measurements described in this section proved problematic when organising site visits to complete this work. This was mainly due to two factors:

- The site operators did not want to be liable for any accidents that may have occurred
- To allow the work to be carried out safely, normal site activities were disturbed

However, these limitations were overcome when sampling on days when the site was normally closed, as described in section 8.3.

8.8.5.2 Pollutant temperature measurement limitations

Temperatures of pollutant emissions were measured mostly during the winter months. This was thought to give a higher contrast between ambient and pollutant temperatures, and thus produce a visible pollutant plume within infrared ranges (Batty, 2010). Despite these efforts, it was not always possible to view a pollutant plume of the TIs produced. This was apparent particularly during shredding activities. As shredding activities are performed on fresh waste, the waste has not yet begun the process of heating which is observed during the main phase of composting (Swan *et al.,* 2003). This may explain why it was not possible to measure pollutant temperatures during shredding activities. Therefore it may be possible that the pollutant temperature is equal to ambient temperature during shredding activities. Additionally, the thermal

imaging camera was focussed on only one part of the activity, where the shredded material exits the machine. Ideally the camera should have been focussed on the whole activity, including where the waste enters the machine, to observe the pollutant temperatures of the whole process. This should be considered when using a TIC in the future.

There are also limitations when operating the TIC itself. Several TICs were used, dependant on model availability. Due to the varying specifications of each TIC used, each TIC would give slightly different temperature readings when measuring the same scenario, as detailed in section 8.4.1. However the differences between each camera are minimal, resulting in a difference of less than 1°C between the different systems. This is less than the accuracy of TICs, which varies from 1 to 2°C, depending on the camera model used. An emissivity value of 0.96 was used based on preliminary experiments as described in section 8.4.1. It is possible that an incorrect emissivity setting has been used, as there is no current knowledge of the ability of a bioaerosol to absorb or reflect radiation, assuming that the observed pollutant plume predominantly consists of bioaerosol components. However, emissivity values can be altered post-measurement within the FLIR QuickReport© software. Figure 8-16 presents the same TI but with two differing emissivity values. The emissivity value of 0.96 used in this study is compared to a lower emissivity value of 0.20.

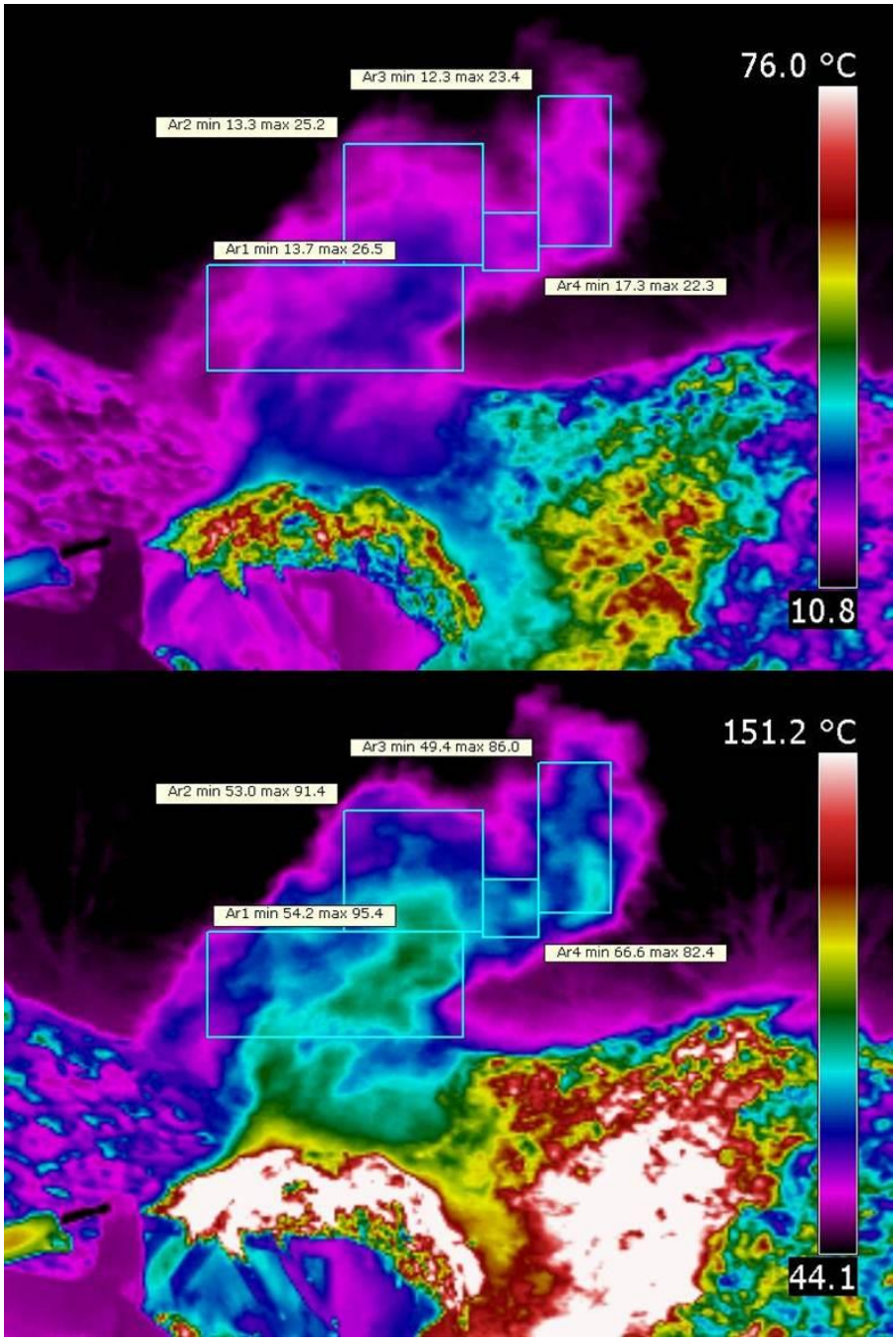

Figure 8-16 Duplicated thermal images of a turning activity with an emissivity setting of 0.96 (top) and 0.20 (bottom). The white and red coloured areas signify where the compost core was exposed. Personal photographs

Figure 8-16 shows that the different emissivity values result in altered temperature ranges from 10.8 to 76.0 and 44.1 to 151.2 °C for the emissivity values of 0.96 and 0.20 respectively, highlighting the importance of using a correct emissivity value. Observing the TI with an emissivity value of 0.20, the

image indicates that the core of the compost reached temperatures of approximately 150°C. This is not possible, as the core of the compost reaches around 55-60°C (Lacey and Crook, 1988), and confirms that low emissivity values are not appropriate when measuring the temperature of bioaerosols. When comparing an emissivity of 0.96 to an emissivity of 1.00 and 0.80, it was observed that the temperature readings altered by up to 11°C (data not shown). This highlights a subtle difference in emissivity can result in a large difference in the temperature reading, emphasising the importance of a correct emissivity value. However, the best emissivity estimate was used based on current knowledge and preliminary tests, and the emissivity can be easily altered at a later date using the FLIR QuickReport© software.

A zero RAT was used in the TICs, based on the assumption that the pollutant plume is opaque and unreflective, as described in section 8.4.1. Similarly to the emissivity values, the RAT can be altered post-measurement within the FLIR QuickReport© software. Altering the RAT from zero to 20 degrees Celsius resulted in a temperature difference of less than 1°C. Alterations in the RAT do not result in such dramatic changes in the temperature measurements as the emissivity setting, however, the most appropriate RAT was used based on current knowledge. Like emissivity, this setting can be altered after the images have been captured.

8.8.5.3 Pollutant exit velocity

As pollutant exit velocity was estimated via visible plume observations, one of the major limitations is related to the visibility of the pollutant plume. In many cases, the pollutant plume was not visible and thus a pollutant exit velocity could not be estimated. As open windrow composting activities are performed outdoors at the majority of facilities, it was assumed that the parts of the plume used to estimate velocity were affected by ambient winds. Therefore, it is highly likely that the presence of ambient wind has affected the results. Additionally the pollutant exit velocity estimations relied upon visual observations of pollutant plume movements and thus were subject to human error. It was difficult to visually follow a singular plume movement between two points whilst

approximating the movement period. If these measurements were to be repeated, it would be useful if points in the pollutant plume could be highlighted, as this would allow more accurate approximations of the plume movement and velocity. It was also not possible to view and estimate pollutant exit velocities from the immediate point of release, due to health and safety implications. Therefore estimations were often based on observations of the plume two or more seconds after release, when plume dispersal had commenced. However the effects of this on the results are thought to be minimal, as the velocity of the plume did not appear to alter during this time.

8.8.5.4 Bioaerosol concentration at source

The sampling equipment set up as described in section 8.6.2 is only capable of sampling emissions at a single point in time and space. It was observed that emissions from shredding and screening activities covered a much larger area when compared to turning activities. Due to equipment availability, it was only possible to sample at one location in the vicinity of the shredding and screening activities. The areas where the compost was deposited into the machine and where the material was removed from the machine were not sampled, as these activities were considered to be similar to the turning removal and turning deposition activities, as described in section 8.6.1. This assumption may be incorrect, as the turning activities are performed on material that is at a different stage in the composting process, and is thus likely to be composed of a different bioaerosol types (Swan *et al.,* 2003). Additionally, measurements taken during the beginning and the end of the main phase may have resulted in concentrations higher or lower than those reported in Table 8-8. Taha *et al.* (2007) concluded that compost age had little effect on bioaerosol concentration. However this was concluded for static compost windrows, not agitated compost windrows, and thus further investigations are required.

There are also limitations with the sampling equipment itself. The filter sampling method has a high LLOD (Pankhurst, 2010). As samples were collected so close to the agitation activities where high bioaerosol concentrations were expected, it was assumed that all concentrations would be above the LLOD.

However zero readings on some replicates were still observed. This may have been caused by blocking of the filter by non-biological components. It may be more suitable if a liquid impingement method was used in the future, to overcome this limitation.

8.8.6 Achievement of objective

8.9 Conclusions

Quantification improvements were made to sensitive model input parameters using novel techniques. Pollutant temperature, pollutant exit velocities and bioaerosol concentrations at the source of agitation activities were quantified to provide more accurate values to use as inputs within the dispersion model. Emission rates were also calculated using the improved parameter quantifications described in this chapter. The novel techniques developed in this chapter can be used others, to further improve the quantification of slected inputs within the dispersion model.

Specifically:

- The temperature of the pollutant plume was measured for the first time using a Thermal Imaging Camera. Measured pollutant plume temperatures were consistently high than ambient temperatures by up to 19°C.
- Pollutant exit velocities were estimated for the first time by observing pollutant plume movements between two fixed points. The estimated pollutant exit velocities were consistently higher than values used within the dispersion model previously, by up to 3 metres per second.
- An existing sampling technique was adapted to allow source concentrations to be measured less than 0.3 metres from agitation activities. These measurements were completed closer to the agitation activity than previous attempts. Generally, the concentrations measured were higher than values reported in the literature, by up to five orders of magnitude.

- Emission rates were calculated by employing equations endorsed by the ADMS model developers, CERC, and using the improved parameter estimates achieved in this chapter. Emission rates ranging $3.60x10^4$ to $1.41x10^7$ CFU/s and $1.53x10^3$ to $2.16x10^6$ CFU/m^2/s were calculated. These calculated emission rates fell within the ranges of emission rates used previously within the dispersion model.

The next chapter describes how the results from this chapter and subsequent chapters (Chapters 3-7) have formed a set of modelling recommendations, to help future modellers to simulate bioaerosol emissions from open windrow composting facilities more accurately.

9 Modelling recommendations

9.1 Introduction

This chapter presents a set of initial modelling recommendations when using the ADMS dispersion model to simulate bioaerosol emissions from open windrow composting facilities in the UK. The recommendations presented in this chapter have been based on evidence from the research completed in Chapters 3, 4, 5, 6, 7 and 8, and have been written to address the objective 'to create best-practice modelling recommendations when using dispersion models to accurately estimate bioaerosol emissions from open windrow composting facilities'. It is assumed that the users of these recommendations are competent users of ADMS, and thus are familiar with the ADMS model interface.

The purpose of the recommendations is to aid model users when using ADMS to predict *Aspergillus fumigatus* concentrations downwind of an open windrow composting facility. This will allow the modeller to produce the most accurate and reliable modelled outputs, based on current evidence, when modelling this scenario.

A sensitivity analysis [SA] specific to the open windrow composting scenario was presented in Chapters 3 and 4. The results from this chapter informed on which model inputs affected the model outputs the most. Therefore particular care should be taken when defining and justifying input values for the sensitive input parameters. Chapters 5,6 and 7 presented a model calibration and validations specific to the open windrow composting scenario. This tested the performance of the dispersion model, in this specific context, providing a set of optimal inputs when using the dispersion model in this specific scenario. These optimum inputs form many of the model input recommendations presented in this chapter. Finally, Chapter 8 presented the results from initial attempts at characterising selected model inputs in the open windrow composting scenario. The initial results from this quantification exercise are also used to provide recommendations in this chapter. Again, it should be noted that the work for Chapter 8 was completed alongside the model tests (Chapter 3, 4, 5,6 and 7),

and the results from Chapter 8 influenced decisions in the model test chapters and vice versa.

It should be recognised that the model calibration and validation tests were completed by comparing modelled outputs to sampled *Aspergillus fumigatus* data. Therefore the recommendations presented in this chapter are made in respect to modelling *Aspergillus fumigatus* concentrations at existing facilities in dry weather conditions. Modelling conditions which vary from this, for example in wet weather conditions or simulating the dispersion of other bioaerosol components, is addressed and discussed further in section 9.5. These recommendations are written with the assumption that the reader is familiar with the ADMS model interface.

9.2 General modelling recommendations

At this time it is recommended that the dispersion model is used to simulate site conditions during periods when measured data has been collected. This will allow the measured and modelled data to be directly compared. This is due to the fact that at present, although greatly improved, there is not enough confidence in the dispersion model outputs, as indicated by the statistical results presented in the model validation chapter (Chapter 6 and 7), when comparing modelled outputs to a set of measured data. Comparing modelled outputs to some sampled data provides an approximate assessment of whether the model is simulating emissions adequately. The measured data should be collected downwind of the composting facility, during agitation activities, allowing the modelled outputs to be directly compared to measured data downwind of the facility. If there is a good correlation between the modelled outputs and the measured data, assessed by calculating the statistics described in section 5.3.3, then the model can be used with increased confidence to simulate emissions over longer time scales and wider spatial areas. For example, initially the model should be used to simulate emissions during time periods when the sampled data was collected, to allow direct comparison between the modelling outputs to sampled data, similarly to the work presented in Chapters 5,6 and 7. If there is a good correspondence between the modelled

and measured data, then the model could be used to simulate emissions over longer time scales.

Ultimately, all model inputs should be coherently justified and entered with care. There has been a distinct lack of model input justification during previous attempts of modelling the open windrow composting scenario, as highlighted in section 2.5, which may have caused substandard modelled outputs when compared to measured data in the past. Additionally, it is recommended that the model is used in the simplest form possible, for the site that emissions are being simulated from. This is due to the fact that there is very limited data regarding the characteristics of bioaerosol emissions from open windrow composting facilities. Once further data has been collected, and the workings of model when applied to this scenario are better understood, it may appropriate to use the advanced model settings.

9.3 Prior to modelling

Prior to modelling *Aspergillus fumigatus* emissions from open windrow composting facilities, certain information and data are required. This includes information on the site and surroundings of the site involved, sampling data, and meteorological data, as detailed below.

9.3.1 Information about the site

The location of the site should be known. This will allow the modeller to assess the site remotely, particularly by using aerial maps. The site surroundings and on-site characteristics can then be assessed, which will aid with some model input decisions. For example, the site surroundings can be assessed to provide a justified surface roughness input based on the predominant wind direction. Observing aerial maps in geospatial software systems such as ArcGIS® (ESRI, 2013) also provides Global Positioning System [GPS] and geometric data for the source of emissions. It also conveys how large a site is, and where the nearest sensitive receptors are located. These aspects are highlighted in section 9.4. These techniques were used throughout the model calibration and validation, presented in Chapters 5,6 and 7. Information associated with the

agitation processes performed on the site is also useful, particularly when justifying source inputs. For example, what agitation activities were taking place, when and where they were performed, and what machinery was used to execute them. This will help to justify certain inputs in section 9.4.

9.3.2 Sampling data

As previously stated, it is recommended that modelled outputs are compared to some measured data to verify the accuracy of the modelled outputs, before completing any further simulations. Ideally, GPS data should be recorded at every sampling location, which is recommended in the sampling protocol (AfOR, 2009). This will aid justifying certain inputs in section 9.4, particularly when setting up the model grid. It is also recommended that if there are any apparent 'zero' values within the sampling data, the modeller should consider altering these values to one lower than the Lower Limit of Detection [LLOD] of the sampling technique used, to represent a 'worst case scenario'. This method was adopted in the model calibration and validation, as described in section 5.2 and Table 6-1, and resulted in the best correspondence between the modelled and measured data.

9.3.3 Meteorological data

Prior to setting up the model, for use in the initial model run, the meteorological data should be edited to include only the dates and times that sampling occurred, similarly to the data used in the model calibration and validation (Chapters 5,6 and 7). Where the resolution of the meteorological data is not detailed enough to provide meteorological measurements at the exact time of sampling, then the next nearest time should be used. For example, if sampling took place at 09:48, and meteorological data was recorded hourly, then meteorological data collected at 10:00 should be used. The characteristics of the meteorological data should also be observed, to aid with the justification of some model inputs, such as the size and position of the modelled grid and what surface roughness should be used, as detailed in section 9.4. If there is good correspondence between the modelled and sampled data, then the model can

be used to predict bioaerosol concentrations over longer time periods and wider spatial scales.

Ideally, meteorological data should be collected on the site that is modelled using a weather station. Meteorological data should be collected as frequently as possible, depending on what the model is used for. The AfOR (2009) sampling protocol states that meteorological conditions should be collected in at least 10 minute intervals when sampling bioaerosols. Weather stations should be set up according to the manufacturer's specifications, and the advice detailed in the sampling protocol (AfOR, 2009). Data collected using this approach should be used wherever possible. However, this data may not be available, particularly when modelling emissions based on older datasets, such as those collected before the sampling protocol existed. It is also appreciated that this type of data may not be available when modelling over longer periods, as the site operators may not agree to a weather station being set-up on site for long periods of time. Moreover, the sampling team may not have access to this equipment for prolonged periods of time. In these circumstances, it is recommended that data collected from nearby weather stations should be used. Such data can be purchased from UK meteorological office (Met Office, 2011a). However, care should be taken when using this type of data, as the meteorological data collection site may be located in an area with different local topography to the composting facility, affecting model output concentrations. This was thought to be the cause of the initial poor correlation between the modelled and measured data in the model validation, discussed in Chapter 7.

9.4 Modelling recommendations

The model input recommendations made in this section are organised based on the input screens in the ADMS model interface.

9.4.1 Setup tab

The setup tab allows the modeller to simulate emissions using more advanced approaches, which requires more complex input data. These options are discussed individually.

The use of the wet and dry deposition modules is not required

Results from the model calibration, presented in section 5.4.2, suggested that the use of the dry and wet deposition modules were not required to provide a good correspondence between the modelled and the measured data. However the results of the sensitivity analysis, presented in Table 4-3, indicated that these modules were very sensitive when modelling the open windrow composting scenario. It is recommended that the dry and wet deposition modules are not used at this present time, particularly as more data is required to use these options, which is not yet available. Further recommendations regarding wet weather conditions are stated in section 9.5.2.

The radioactive decay, plume visibility, odours, chemistry, coastline and fluctuations options are not relevant to this scenario, as highlighted in Table 4-1. Therefore it is recommended that these options are not used when estimating *Aspergillus fumigatus* concentrations from open windrow composting facilities. However, ADMS is a complex model with multiple options, some are appropriate and others are not, depending on the purpose of the model simulation. Therefore some of these advanced options may relevant to some open windrow composting scenarios. For example, it may be necessary to use the coastline or complex terrain module if the open windrow composting facility is located on complex terrain or near to a coastline. However these options were not assessed or tested during this study, and therefore recommendations cannot be made regarding these options based on the work completed in this study.

The use of the buildings module is not necessary

The results of the model validation indicated that using the buildings module worsened the fit between the modelled and the sampled data (section 7.2.2). Therefore it is recommended that, based on this information, the buildings options should not be used when modelling this scenario. However, if a poor correspondence between the modelled and measured data is observed when modelling emissions from a site located close to buildings, then this option

should be tested. Aerial maps can be used to estimate the size of buildings when defining them within the dispersion model, as described in section 7.2.

The puff module was not a sensitive input parameter when using the ADMS dispersion model to simulate the open windrow composting scenario, as detailed in Table 4-3. Therefore it is recommended that this option is not used at this stage.

The setup tab also allows the user to include additional input files in the model, which are usually associated with the more advanced options. Therefore the use of the additional input files will not be required when modelling the open windrow composting scenario. However, an additional input file may be required when modelling low wind speeds. If wind speeds of less than 0.75 m/s are included in the meteorological file, then the model will not simulate emissions in those conditions (CERC, 2010b). If the 'CALMS' additional input file is used then the model will simulate conditions in lower wind speeds. If the 'CALMS' option is required, then it is recommended that the default options are used, as this option provided the best fit between the modelled and the sampled data during the model calibration (Table 5-5). However, to reiterate, the meteorological file should be carefully checked prior to using this option, to ensure that the use of this option is necessary.

9.4.2 Source tab

An area source type, representing the size of a composting windrow should be used to represent the source of the emission

The results of the model calibration indicated that an area source should be used to represent bioaerosol emissions during agitation activities performed at open windrow composting facilities (Table 5-5). The results of the model calibration also suggested that the size of the area source should represent the size of an average windrow at the composting facility being modelled. This was confirmed by the results of the model validation, presented in section 7.3.2. The size of a composting windrow can be measured directly on site, or estimated remotely by measuring the size of the windrow from recent aerial maps, using

geospatial analysis software such as ArcGIS® (ESRI, 2013). If a grid based on GPS points is used, then the source geometry should reflect this positioning system, as described in more detail in the grids section below (section 9.4.5). Larger and smaller source sizes, with differing emission rates were tested in the model calibration, as highlighted in Figure 5-6, but this representation provided the best correspondence between the modelled and measured data, in both the model calibration and validation chapters. Therefore, by representing the source in this way, the different agitation activities are not represented by multiple source types but in fact by the value of the emission rate. For example, a higher emission rate will represent more agitation activities. However, this notion has not been tested fully.

An emission rate proportional to the mean average bioaerosol concentration data should be used until further investigations regarding the emission rate have been completed

The corresponding emission rates used for this type and size of source used throughout the model calibration and validation were proportional to the mean average measured *Aspergillus fumigatus* concentrations collected at the site simulated. To reiterate, the mean measured concentration of *Aspergillus fumigatus* used to validate the model decreased by 75% from the measured data used to complete the model calibration. Therefore the emission rate was also decreased by 75% from $9x10^6$ to $2x10^6$ CFU/m^2/s, as described in section 7.4. Units of g/m^2/s were used as a proxy to CFU/m^2/s as Colony Forming Units [CFUs] are not available within the model interface. At this time it is recommended that the same technique is adopted whereby the mean measured *Aspergillus fumigatus* concentrations collected downwind of the modelled site are compared to the measured concentrations of the data used in the model calibration. The emission rate should also be increased or decreased proportionally from the emission rate used in the model validation. For example, the mean measured concentrations should be compared to those used in the model validation. If on average the mean measured concentration has increased by 5%, then the emission rate should be increased proportionally, by

5% from $2x10^6$ CFU/m^2/s (the value used in the model validation). However, a more precise technique may be available in the future. For example, Chapter 8 detailed how bioaerosol concentrations measured at the source of the pollutant emission can be used to calculate an emission rate. These results have not yet been tested within the dispersion model, therefore this technique is not recommended at this stage, but should be considered in the future after completing further tests, as described in section 9.6.2.

A source height of 2.65 metres should be used

The optimal source height determined from the completion of the model calibration was 2.65 metres, as highlighted in Table 5-5. This value was also used in the model validation (Table 6-1). Therefore it is recommended at this stage that a source height of 2.65 metres is used based on these results. However, it should be reiterated that the source height is a sensitive parameter within the dispersion model when used to simulate the open windrow composting scenario, as highlighted in Table 4-3. Therefore it is important that the correct height is used within the model to obtain the most accurate model outputs. Therefore the modeller may find it appropriate to use an alternative source height to represent the site that is simulated. Providing this value is well justified, then this acceptable, although it is recommended that the outputs produced when modelling with a source height not equal to 2.65 metres are compared to the outputs produced when modelling with a source height of 2.65 metres. This will allow the modeller to evaluate which set of modelled outputs provide the best correspondence to the measured data, similarly to if the coastline or buildings options are used, as described above.

A pollutant exit velocity of 2.95 m/s and a pollutant temperature of 29°C should be used

The optimal pollutant exit velocity and pollutant temperature provided from the model calibration was 2.95m/s and 29°C respectively, as highlighted in Table 5-5. These values also provided the best fit between the modelled and sampled data throughout the model validation, although a scenario specific pollutant temperature was also tested. These values were based on initial measurements

as detailed in sections 8.4.2 and 8.5.2. However, there is scope to improve and expand on the initial measurements that were taken, as detailed in section 8.8.5, which may influence model inputs in the future, particularly during additional model validation tests, as discussed further in section 9.6.3.

A pollutant specific heat capacity of 1519 J/°C/kg and a pollutant molecular mass of 28.996g should be used

These were the optimal values that provided the best correspondence between the modelled and measured data in the model calibration, as highlighted in Table 5-5. These values were also used in the model validation. Therefore it is recommended that these input values are used when modelling this specific scenario.

All other parameters within the source tab should be retained at the model default values at this stage, based on the results of the model calibration and validation. A new pollutant, as defined within the 'palette of pollutants' should be used, maintaining the model default values. This method was used throughout the model calibration and validation. As the use of the dry and wet deposition modules are not recommended at this stage, it is not necessary to define any parameters within the palette of pollutants, as this will not alter the model output (CERC, 2010b; Johnson, 2011b).

9.4.3 Meteorology

Use reliable, high resolution meteorological data

As already stated in section 9.3.3, the meteorological data used within the dispersion model should be from a reliable source, and of high resolution. Meteorological data can be entered directly within the model interface or attached as a separate file. As a minimum requirement of the dispersion model, meteorological files must contain at least the wind speed, wind direction and either; a reciprocal of the Monin-Obukhov length, the surface sensible heat flux or the cloud cover and time and date (CERC, 2010b).

Determine the surface roughness by observing the dominant wind direction

The dominant wind direction should be observed, to aid with the justification of the surface roughness used within the dispersion model. The surface roughness was discovered to be a slightly sensitive input parameter in the context of the composting scenario during the sensitivity analysis, and thus it is important that the correct surface roughness is used within the dispersion model. For example, if the predominant wind direction is from the east, then the terrain and land use type to the east of the site being modelled should be observed and used to determine what surface roughness is used. The appropriate land use or terrain type can be selected from the surface roughness drop-down menu in the model interface. This technique was practised the model calibration, and provided a good fit between the measured and the modelled data, and thus was applied to the model validation. The wind speeds within the dispersion model should also be observed to obtain whether the use of a 'CALMS' additional input file is required.

All other values within the meteorology tab should remain at their default values. The model user may wish to change the site latitude, however this option was discovered to be not very sensitive, or not very sensitive at all during the sensitivity analysis (Table 4-3) and thus it is not necessary to change this option when modelling bioaerosol emission from open windrow composting facilities in the UK.

9.4.4 Background information

The backgrounds option should be used, based on the concentrations of samples collected upwind of the composting facility being modelled

The backgrounds option was tested as part of the model calibration. Using this option resulted in an improved fit between the modelled and sampled data. Therefore, based on this evidence, it is recommended that the backgrounds option is used. During the model calibration, several background inputs were tested as highlighted in Table 5-5 and Figure 5-3, based on the concentrations

of measurements taken upwind of the site sampled. As some ‘zero’ values were observed at upwind locations, and all ‘zero’ values were altered to one lower than the LLOD as described in section 5.2, a background option pertaining to one lower than the LLOD was used. Therefore it is recommended that a background, based on concentrations collected at a location upwind of the site, is used as the backgrounds value in the dispersion model. This value can be entered by hand, for the relevant pollutant, within the model interface.

9.4.5 Grids options

The grids option within the dispersion model allows the modeller to define where the output concentrations will be calculated by the model (CERC, 2010b). Therefore the grid used should be applicable for the scenario in which the modeller is simulating. It should be large enough to allow all required output concentrations to be calculated in the desired locations, but not too large, so that a good resolution is retained.

Use GPS data where possible

During the model calibration and validation stages (Chapters 5,6 and 7), a Cartesian coordinate system was adopted, based on the GPS points of the sampled data. Specified output points were defined, so that the modelled outputs could be directly compared to the sampled data. This approach is recommended to allow direct comparison between the modelled and sampled data, in the initial model run. However, the modeller may wish to use another approach, such as the Polar coordinate system, which is acceptable, providing that the measured data is compared directly to the modelled outputs, at the same location and time. After the initial model run, the modeller may also want to simulate conditions in locations where sampled data was not collected. In this case additional specified points can be added, using GPS points collected on-site or from aerial photographs using geospatial software, or a wider grid may be used, whereby output concentrations are calculated at regular or variable intervals across the simulated space. Any approach is acceptable, providing that it is justified for the circumstances that the model is being used.

9.4.6 Model output options

A new pollutant output should be defined for the pollutant simulated. The units of output should correspond to the proxy units used for the emission rate in the source tab. For example if units of $g/m^2/s$ were used for the emission rate then g/m^3 should be used as unit for the model output.

A short term averaging time of x minutes should be used initially (where x is equal to the sampling time)

During the model calibration, different averaging times were tested as highlighted in Table 5-5. A short term averaging time of 30 minutes provided the best correspondence between the modelled and measured data, which was used in the model validation. This was based on the sampling time used to collect the measured data (30 minute sampling time, as described in section 5.2), following the advice of the model developers (Lad, 2012a). This was the appropriate averaging time for the modelling application, as modelled outputs were being directly compared to sampled data. Therefore an averaging type and time corresponding to the sampling time should be used in the initial model run. If a different sampling time is used to collect the measured data, then the averaging time should be changed accordingly, corresponding to the advice of Lad (2012a). All other options should remain at the default values. It is possible to model short term averages over long time scales, as detailed in the model user guide (CERC, 2010b). However, the modeller may find it appropriate to use a long term average, over a longer averaging time. However, this has not been tested in this study, and if completed should be used alongside, and compared short term calculations where possible.

9.5 Other considerations

The recommendations listed in section 9.4 are based on modelling *Aspergillus fumigatus* concentrations, from existing open windrow composting facilities in dry weather conditions. This section provides suggestions as to how a modeller should approach situations that slightly differ from these conditions. It should be

noted that these suggestions have not been tested, and should be used with caution.

9.5.1 Modelling other bioaerosol components

The model calibration and validation were completed by comparing modelled outputs to sampled *Aspergillus fumigatus* concentrations, as described in section 5.2 and 6.2, hence why the recommendations detailed above are for when modelling *Aspergillus fumigatus* concentrations from open windrow composting facilities. However, as the use of the wet and dry deposition options are not recommended, the definition of the pollutant in the 'palette of pollutants' is not required, as stated in section 9.4.2. Therefore, there is nothing defined within the dispersion model that is specific to *Aspergillus fumigatus*. Consequently, theoretically, it should be adequate to use the settings detailed above for other bioaerosol components, such as Gram-negative bacteria. However, it should be recognised that different bioaerosol components will be emitted in different proportions during different agitation activities. For example, when measuring bioaerosol concentrations at the source, as described in section 8.6, generally concentrations of Total Bacteria were higher than concentrations of Gram-negative Bacteria and *Aspergillus fumigatus.* The emission rate can be altered to reflect these differences, although this has not been fully tested. To reiterate, modelled outputs should be compared to measured data, to test the performance of the dispersion model.

9.5.2 Modelling in wet meteorological conditions

Although at present it is recommended that that the wet and dry deposition modules are not used. If the modeller requires wishes to simulate bioaerosol emissions and dispersal conditions within wet meteorological scenarios, then the wet deposition module should be used. The wet deposition module accounts for material lost within the pollutant plume from 'washout' caused by precipitation (CERC, 2010b). The wet deposition module was a very sensitive model input parameter, and thus has a large affect on the modelled output concentrations. However, care should be taken when interpreting the modelled outputs when using this option, as it has not yet been fully tested. Testing this

option has not been possible as sampling is completed in dry weather conditions (AfOR, 2009). Therefore there is no dataset in existence to validate the accuracy of the wet deposition module.

9.5.3 Modelling on sites where there is no measurement data

At present, it is recommended that initially, the modelled outputs are compared to measured data to test the performance of the model. If successful, then the model can be used over broader spatial and temporal scales. However, this approach is not possible if there is no measured data at the site modelled, such as at a site willing to expand, or a site that does not yet exist. In these cases it is recommended that the model is setup to represent the proposed site as closely as possible. When justifying more site-specific model inputs, such as the emission rate, it is recommended that data and information from an existing site should be used to back calculate an emission rate. The existing site should be of similar size, and located within similar topographical conditions to the proposed site. This method has not yet been tested, and thus should be used conservatively.

9.6 Future considerations

As there are still many tests to be completed when modelling bioaerosol emissions from open windrow composting facilities, for example modelling in wet weather conditions, this section summarises any work that could be completed to enhance the recommendations and suggestions presented in this chapter.

9.6.1 Advanced model options

As detailed in section 9.4.1, complex terrain or coastline options may be required if the facility being simulated is located on, or near to, terrain that has a gradient of more than 1:10, or the coast. However these options have not yet been tested within the open windrow context, and should be used cautiously until further validation tests are completed. To test these options, it is suggested that a model calibration and validation, similar to those presented in Chapter 5,6 and 7, is completed, to test model performance in these specific conditions. To

allow these tests to be completed, measured data from relevant open windrow composting facilities is required.

As described in section 9.5.2, the wet deposition module is a sensitive input parameter and should be used during wet weather conditions, to simulate pollutant ‘washout’ caused by precipitation (CERC, 2010b). However, the use of this option has not yet been validated, primarily because current sampling techniques cannot be used in wet weather conditions (AfOR, 2009). Therefore, at present, there is no sampled data that has been collected during wet weather conditions, and thus it is not possible to compare modelled outputs to measured data for validation. Consequently, research is required to develop, or adapt an existing sampling technique to allow bioaerosol data to be collected during wet conditions. When this has been completed, and the necessary data has been collected, then the use of this option can be validated.

9.6.2 Pollutant emission rate

At present the model recommendations suggest that emission rates are proportional to measured data, as described in section 9.4.2. Initial emission rate calculations were completed based on measured data collected at the source of specific agitation activities, as described in Chapter 8. This method could be used to provide an accurate emission rate for use within the dispersion model. However this has not yet been tested, and requires further research. Ideally concentration measurements at the source of the agitation activity would have been taken alongside measurements downwind of the activity, allowing the calculated emission rate to be validated. This was not possible in this study due to time and equipment constraints. Using such measurements in the dispersion model may also have implications on the geometry of the source. For example, as these emission rates were calculated from data collected during individual agitation activities, it may be more appropriate to assign smaller source geometries to the calculated emission rates. Therefore a smaller area source may be required, and should be considered and tested in the future.

9.6.3 Pollutant temperature, pollutant exit velocity and other source properties

Chapter 8 described the first attempts at measuring the pollutant temperature and exit velocity. Although improvements to the methods used to collect this data can be completed, as discussed in section 8.8.5, they may be used to provide more accurate model inputs. These parameters are sensitive in the composting context, so it may be required that site specific measurements of these parameters are required in the model. Results from the model calibration and validation indicated that site specific measurements are not required. However it should be appreciated that the model calibration and validation were competed using data collected from just two facilities in the UK, and further model validation studies are required to confirm these results.

9.6.4 Averaging times

The recommendations presented above currently state that a short term averaging time of 30 minutes should be used when modelling the open windrow composting scenario. This method is not ideal when modelling the overall bioaerosol emissions from a composting facility over a long period of time, for example, a year. This is due to the large number of outputs generated, and the large amount of data analysis associated with it. Therefore, it may be more appropriate to model with longer averaging times. However, the use of this option has not been fully tested. It was considered during the model calibration, as highlighted in Figure 5-6 and Table 5-5, but resulted in an exacerbated correspondence between the modelled and the measured data. However, the sampled data, and thus meteorological data was collected over a short period of 15 different days, which may explain why this option was not successful. Modelling meteorological data collected over long periods, such as a year or more, would be more suitable. However, as it is not yet practical to continuously monitor bioaerosol concentrations, it would be difficult to test whether the modelled outputs are representative of actual bioaerosol concentrations.

9.6.5 Other considerations

At present, the set of modelling recommendations presented in this chapter is only suitable to model *Aspergillus fumigatus* concentrations using ADMS. It would also be desirable to model the dispersion of other bioaerosol components, as described in in section 9.5.1. This can be tested by performing additional model calibration and validation tests, using the methods presented in Chapters 5,6 and 7, using measured data for other bioaerosol components, such as Total bacteria. This would enable exposure levels to be estimated for different bioaerosol components, allowing researchers to assess the exposure levels of different bioaerosol components and the onset of associated potential negative health effects.

A similar set up, based on the recommendations presented above may also be suitable when using alternative dispersion models, such as AERMOD. To test this notion, similar model calibration and validation tests, as presented in Chapters 5, 6 and 7 , could be applied to other dispersion models to test this notion.

Additionally, the model cannot yet be used with confidence to estimate future bioaerosol emissions, which is useful for new sites and sites wishing to expand, as the sampled data does not yet exist. This is particularly useful during the site permitting process, as it has the potential to strengthen a sites application, as the site may be able to prove that certain concentrations will not be exceeded at the nearest sensitive receptors. Initial suggestions were made in section 9.5.3, but further tests are required to test the validity of these suggestions. To test this notion, it is suggested that a 'before and after' analysis is completed, whereby:

- emissions are estimated from the proposed site following the suggestions completed in section 9.5.3 ('before' scenario)
- once the proposed site is operational, emissions are estimated again, following the recommendation presented in this chapter ('after' scenario)
- both sets of modelled outputs are compared to evaluate how well emissions were estimated in the 'before' scenario

If the outputs correspond well, then these results would support the suggestions presented in section 9.5.3.

9.7 Conclusions

This chapter has presented the first set of modelling recommendations when using ADMS to model bioaerosol emissions from open windrow composting facilities in the UK. Overall, it was recommended that:

- The wet and dry deposition, and buildings options are not used
- The source is represented as area, with geometry representing the size of a compost windrow on the site being modelled
- The emission rate is back calculated to correspond proportionately to measured bioaerosol concentration measurements
- A source height of 2.65 metres is used
- The pollutant exit velocity and pollutant temperature used is 2.95 m/s and 29°C respectively
- The backgrounds option is used
- Good quality meteorological data is used, preferably collected on the composting facility that is modelled
- The surface roughness, grids options and any additional options, such as ‘CALMS’ is based on information from the meteorological file

It was also recommended that initially the modelled outputs are compared to some measured data, to test the performance of the model, before simulating emissions over wider time and spatial scales. These recommendations will aid future users of the ADMS model when modelling bioaerosol emissions in the open windrow composting context.

The next chapter summarises discusses the achievements and limitations of this project as a whole, and recommendations for future work are suggested.

10 Final outcomes

10.1 Reminder of the project aim

This project aimed to improve the confidence in simulated output concentrations, when using dispersion models to estimate bioaerosol emissions and dispersal from open windrow composting facilities, focussing on emissions from agitation activities. Dispersion models have become an increasingly sought after tool when assessing bioaerosol concentrations in the vicinity of open windrow composting facilities, due to the limitations associated with current sampling methods. For example, current sampling methods are very time consuming and costly, and provide only a snapshot of emissions spatially and temporally. Dispersion models have the potential to overcome the limitations posed by current sampling methods. However there has been modest progress when applying dispersion models to this complicated scenario over the last decade, as a result of limited data and knowledge, primarily due to the complex nature of this environment.

The aim of this project was:

To improve the confidence in model outputs when using dispersion models to estimate bioaerosol concentrations downwind of emissions from open windrow composting facilities.

This aim was addressed by defining several objectives, designed to confront the gaps in knowledge associated with this subject field. The work presented in Chapters 3 to 9 delivered the work required to fulfil these objectives. The key findings from each chapter are summarised in section 10.2. Section 10.3 addresses whether each objective was achieved, and thus whether the overall aim of this project was achieved.

10.2 Key results, findings and implications

10.2.1 Chapters 3 and 4 – Sensitivity analysis

A sensitivity analysis [SA] was completed in Chapters 3 and 4 to address the lack of data surrounding the open windrow composting scenario. Chapter 3

presented an initial SA screening stage, and Chapter 4 used the results from the screening stage to perform the main SA. As there are so many undefined and unjustified model inputs input parameters in the dispersion model, when modelling the open windrow composting context, the SA was completed to provide an order of prioritisation when quantifying model input parameters. It also provided an order in which to complete the model input parameter adjustments throughout the model calibration. The main findings of the scenario specific SA were:

- The Priestly-Taylor parameter, surface albedo, relative humidity and cloud cover parameters were not sensitive
- The majority of parameters associated with the rudimentary elements of the source of the emission were very sensitive or slightly sensitive
- The wet and dry deposition modules were very sensitive
- The puff module, and all associated model inputs, were not sensitive

Prior to this analysis, modellers were not certain of what model inputs were the most critical within the dispersion model, when modelling the open windrow composting context. Taha *et al.* (2007) suggested that bioaerosol aggregation properties should be considered when modelling bioaerosol dispersion, as aggregation can affect factors such as pollutant gravitational settling rates. As there was limited knowledge regarding the aggregation properties of bioaerosols, it was not possible for Taha *et al.* (2007) to include these effects within the dispersion model. Tamer Vestlund (2009) completed initial work to quantify bioaerosol size and aggregation properties, using a Scanning Electron Microscope [SEM], which is very costly and time consuming method. However, the results of the SA presented in this study revealed that the pollutant particle size and density properties were not very sensitive in the open windrow composting context. The completion of this SA has indicated which model input parameters are definitely sensitive allowing quantifications to be made to the most sensitive input parameters.

10.2.2 Chapters 5, 6 and 7 – Model calibration and validation

The model calibration and validation presented in Chapters 5, 6 and 7 were designed to test the accuracy of the dispersion model outputs when compared to sampled data, using different model inputs relevant to the open windrow composting scenario. The adjustments made in the model calibration were made within the ranges of the input parameters defined for the SA (Table 4-1). The order of adjustments to the input parameters was completed based on the order of sensitivity and level of existing knowledge of the parameters (Table 5-1). Additionally, results from selected input parameters quantifications (Chapter 8) were used to justify modifications in the model calibration, and additional tests performed as part of the model validation. The results from these chapters showed that the best correspondence between the modelled and measured data was achieved when:

- Agitation activities were represented as area sources, with a geometry representative of the area of a compost windrow at the site that is simulated
- Advanced model options such as the wet and dry deposition and buildings modules are not used
- An emission rate proportional to average measured pollutant concentrations is used
- A pollutant temperature and pollutant exit velocity of 29°C and 2.95 metres per second was used
- The backgrounds option was used

The statistical analysis indicated that the model was not successfully validated in the open windrow composting context, as highlighted in Table 7-5 and Table 7-6. However, the results from the model validation show that the model is overestimating measured concentrations by less than one order of magnitude. Generally in previous studies, the model was underestimating sampled concentrations by at least an order of magnitude, as discussed in section 7.5.1. Therefore the results from this validation study show that the accuracy of the modelled outputs has improved.

10.2.3 Chapter 8 – Selected model input parameter quantification improvements

The results from the SA (Chapters 3 and 4), were used to determine which model input parameters would be initially improved quantitatively. Initial measurements of the pollutant temperature, pollutant exit velocity, and concentration of particular bioaerosol concentrations at the source of different agitation activities were completed for the first time. These measurements were completed due to the distinct lack of model input justification in other open windrow composting modelling studies, as highlighted in sections 2.5 and 8.2. This information was also used to calculate emission rates for the selected bioaerosol components. The main findings were:

- The measured pollutant temperature was consistently higher than the measured ambient temperature
- The measured pollutant exit velocity ranged from 0.3-3.0 m/s
- The bioaerosol concentrations measured at the source of the agitation activities, were generally higher than the bioaerosol concentrations reported in other measurement studies
- The calculated emission rates ranged between $3.60x10^4$ to $1.41x10^7$ CFU/s for a point source and $1.53x10^3$ to $2.16x10^6$ CFU/m^2/s for an area source. These values fall within the ranges of emission rates used in previous studies where bioaerosol emissions from open windrow composting facilities have been modelled.

The work presented in this chapter was completed alongside the work completed in Chapters 3 to 7. This is illustrated in Figure 10-1.

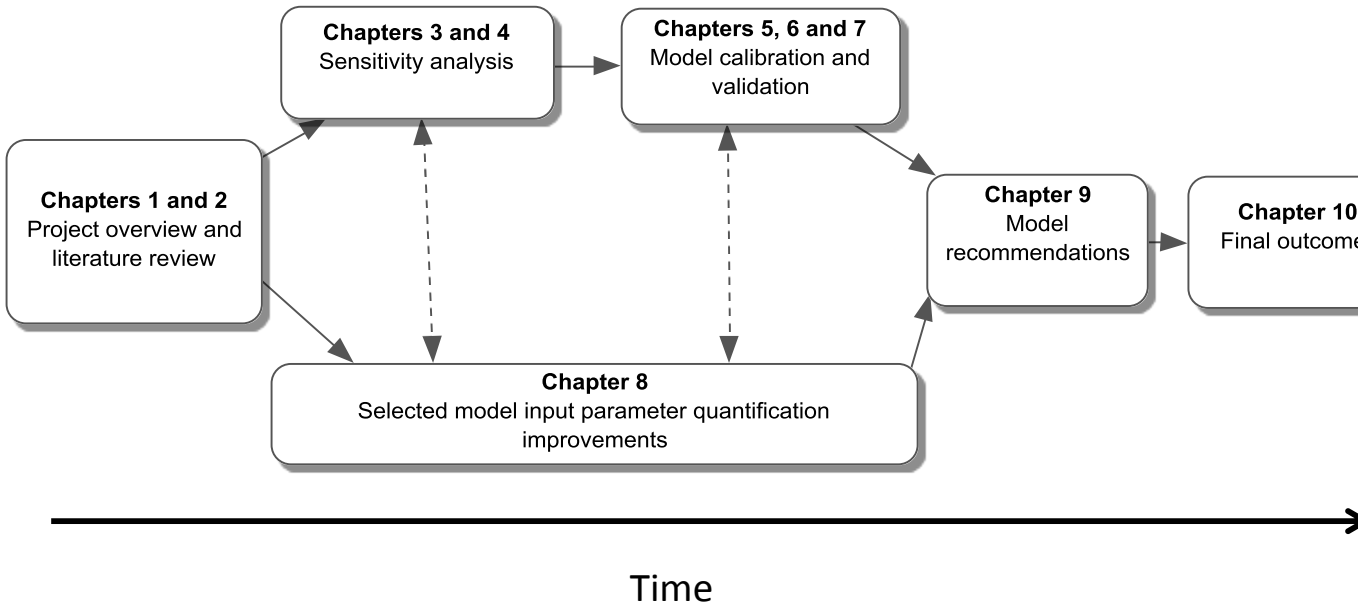

Figure 10-1 Conceptualisation of how the work presented in this thesis was completed over time, highlighting how the results from each chapter influenced others.

The emergent findings from this chapter influenced decisions and justifications in Chapters 3 to 7 and vice versa. Referring to the blue letters in Figure 10-1:

a. Initial observations of site activities helped to define selected parameter input ranges in the SA, such as source height and dimension ranges in Table 4-1
b. The results of Chapter 3 and 4 (Table 4-3) defined what input parameters were quantified in Chapter 8, so that only sensitive inputs were defined
c. Initial results from Chapter 8 were used to justify certain model input value adjustments in Chapter 5. For example, emergent results indicated that the pollutant temperature was approximately 20-30°C. Therefore adjustments completed in Chapter 5 were justified using information from chapter 8 (Table 5-5).

d. The results from Chapters 5, 6 and 7 showed that bioaerosol emissions are best represented as area sources. Therefore emission rates were calculated for area sources (section 8.7)

10.2.4 Chapter 9 – Modelling recommendations

Chapter 9 drew together all the results from Chapters 3 to 8 to produce an initial set of modelling recommendations. This was designed to help users of the ADMS when modelling *Aspergillus fumigatus* concentrations emitted from open windrow composting scenario. In summary, it was recommended that:

- Initially the modelled outputs should be compared to a set of sampled data to provide a quick model validation test, to ensure that the model is performing accurately
- All inputs are well justified
- The open windrow site surroundings and measured data are assessed prior to modelling, to gauge certain input options such as grid sizes and surface roughness
- Good quality, high resolution meteorological data is used, ideally collected on the site of the simulated facility
- Additional input options are not used, with the exception of the 'CALMS' option, if there are wind speeds of less than 0.75 metres per second present in the meteorological data
- Agitation activities are modelled as area sources, pertaining to the size of a composting windrow on the site that is simulated
- Initial values of 29°C, 2.95 metres per second and 2.65 metres are used to represent the pollutant temperature, pollutant exit velocity and height of the emission respectively
- Surface roughness is predicted based on the land use upwind of the facility modelled
- The backgrounds option is used, using a value based on concentration data collected upwind of the facility
- A grid large and of high enough resolution for the modelling application is used. Initially, it is recommended that GPS information from the sampling

points is used, to allow direct comparisons between the measured data and the modelled output concentrations

- Initially, a short-term averaging time should be used, pertaining to the sampling time used to collect the measured data. If modelling over long timescales, justified long-term averaging times may be considered, alongside short-term calculations

Suggestions when modelling other bioaerosol components, or using other dispersion models, or modelling emissions from sites that do not yet exist were also provided.

10.2.5 Pollutant emission rate

The pollutant emission rate is the most sensitive parameter within the dispersion model, as altering this parameter will cause a proportional change in the output concentration. For example, if the emission rate is doubled, then the output concentration is also doubled (Johnson, 2011a). As the sensitivity of the emission rate was already known, this input parameter was not included in the sensitivity analysis (Table 4-1). A large range of emission rates have been used in dispersion models when predicting bioaerosol concentrations from open windrow composting facilities prior to this study, spanning from $6.0x10^{-6}$ $g/m^2/s$ (ADAS, 2005) to $6.7x10^{10}$ particles per second (Millner *et al.,* 1980), as highlighted in Table 2-6. Recently, an unpublished report was completed by the Environment Agency (2012). Point source emission rates were back calculated from 42 sets of measured *Aspergillus fumigatus,* Mesophilic Bacteria, and Gram-negative Bacteria data, collected downwind of 32 different open windrow composting facilities. The back calculated emission rates varied between approximately $1x10^4$ – $1x10^9$ CFU/s, mean averaging at $8x10^6$, $6.6x10^6$, and $5.0x10^5$ CFU/s for *Aspergillus fumigatus,* Mesophilic Bacteria, and Gram-negative Bacteria respectively (Environment Agency, 2012), falling within the ranges previously used in dispersion models (Table 2-6). The mean average emission rates reported in the Environment Agency study could provide a reasonable estimate of bioaerosol concentrations downwind of open windrow composting facilities, if used within dispersion models (Environment Agency,

2012). In this project, several emission rates were tested, within the large range reported in the literature, throughout the model calibration (section 5.3.2 and Table 5-5). An optimal emission rate of $9x10^6$ was provided by the model calibration, and tested in the model validation alongside an emission rate of $2x10^6$ CFU/m^2/s, adjusted proportionately to the mean measured concentration data. The emission rates fall within the ranges of those used in previous modelling studies, and corresponds well to the mean average back calculated emission rates reported in the unpublished Environment Agency report (Environment Agency, 2012). At present it is recommended that an emission rate proportional to the mean measured concentration data should be used within ADMS, based on the results presented in the model calibration and validation (section 9.4.2). However, in Chapter 8, emission rates were calculated based on bioaerosol measurements taken within <30cm of agitation activities for the first time (section 8.7). The calculated emission rates varied between $1.53x10^3$ - $2.16x10^6$ CFU/m^2/s and $3.60x10^4$ - $1.41x10^7$ CFU/s, which fall within the range of emission rates used in previous studies. However, it is not recommended at this stage that measurement methods are used to calculate emission rates for use within dispersion models. This is because the emission rate measurements detailed in Chapter 8 have not been tested within the dispersion model. Ideally, the measurements taken at the pollutant source (and used to calculate an emission rate) would have been completed alongside measurements taken downwind of the agitation activities. However this was not possible due to time and equipment constraints. If completed, this would have allowed modelled outputs, generated by using the calculated emission rate in ADMS, to be compared to the measured downwind concentrations, testing the validity of modelled outputs when using measured emission rates. Overall, despite the advances made within this project and the Environment Agency study (Environment Agency, 2012), there are still some uncertainties on what emission rate(s) should be used within the dispersion model to provide the most accurate bioaerosol concentration estimations. Suggestions for future research work to overcome these uncertainties are provided in section 10.6.

10.3 Objective achievement and contributions to knowledge

10.3.1 Objective 1 - Sensitivity analysis (Chapter 3 and 4)

Chapters 3 and 4 provided the first SA, in the context of bioaerosol emissions from open windrow composting, on any dispersion model. It also presented the first evidence of critical thought regarding what input parameters and ranges are relevant in this specific context (Table 4-1). Therefore, objective 1, “to perform a sensitivity analysis, specific to the scenario of bioaerosol emissions from open windrow composting facilities, to determine which input parameters affect the model output concentrations the most” was fulfilled.

By completing this objective, it is now established which ADMS model input parameters are the most crucial in the open windrow composting context. This has provided a significant contribution to knowledge by improving the understanding of how the ADMS model operates when applied to this specific scenario. The results from this SA have influenced decisions in succeeding chapters, by providing an order of prioritisation when adjusting model inputs in the model calibration (Chapter 5) and improving the quantification of model inputs (Chapter 8). Additionally, it has provided precedence to future input parameter quantification improvements, preventing non-sensitive parameters from being quantified, potentially reducing sampling times and costs.

10.3.2 Objective 2 – Model calibration and validation (Chapters 5, 6 and 7)

Although many model validation studies have been performed on ADMS prior to this study, the validation studies have been completed in conditions not applicable to the open windrow composting scenario. Therefore, prior to this study, the ADMS model had not been fully tested in the open windrow composting scenario. This formed the objective “to complete a model calibration and validation, in the context of bioaerosol emissions from open windrow composting facilities, using existing sets of measured data” which was fulfilled in Chapters 5, 6 and 7. Therefore Chapters 5,6 and 7 presented the first model

calibration and validation on the ADMS dispersion, specific to bioaerosol emissions from open windrow composting facilities.

The optimal inputs gained from the model calibration were applied to the model validation. The model validation tested the optimal model set up at a different composting site, by comparing modelled outputs to a set of measured data. The statistical analysis from the model validation indicated that the model was still not performing well in the open windrow composting contest. However, the model was estimating average measured data within one order of magnitude. This is a significant improvement on previous modelling studies, as generally concentrations were underestimated by at least one order of magnitude. Therefore this study has presented the most accurate modelled outputs when using a dispersion model to simulate the open windrow composting context. Due to this significant improvement, the dispersion model can be used with more confidence in this specific scenario. This has significant future implications, as now the model can be used more accurately to predict bioaerosol concentrations over longer timescales and spatial scales. This is discussed further in section 10.4.

10.3.3 Objective 3 – Selected model input parameter quantification improvements (Chapter 8)

Objective 3 was to “collect data, using novel techniques and existing data collection methods if possible, to improve the knowledge of selected dispersion model inputs, in the open windrow composting context, to provide more accurate modelled output concentrations”. This was addressed in Chapter 8. Chapter 8 provided the first measurements of:

- The pollutant temperature
- The pollutant exit velocity
- The concentration of selected bioaerosol components

in the open windrow composting context

These measurements were completed during different seasons and at the source of different agitation activities. The pollutant exit velocity, bioaerosol

concentration measurement results, and estimated dimensions of the agitation activities were used to compute the first direct calculations of the pollutant emission rate in this unique context.

This has provided improved and justified model inputs to use within the dispersion model for the first time. It has also provided the modeller with methods of justifying inputs when using the dispersion model to simulate bioaerosols in the open windrow composting context.

10.3.4 Objective 4 – Modelling recommendations (Chapter 9)

Chapter 9 addressed objective 4, “to create best-practise modelling recommendations when using dispersion models to accurately estimate bioaerosol emissions from open windrow composting facilities”. This objective was achieved by compiling all of the results from preceding chapters (Chapters 3, 4, 5, 6,7 and 8). This has formed the first set of modelling recommendations when using the ADMS dispersion model to predict bioaerosol concentrations from open windrow composting facilities. Although many additions and improvements can be made to these recommendations once further work has been completed, these recommendations have provided modellers with guidance when modelling this specific scenario for the first time. Therefore the model can now be used with more confidence, when estimating bioaerosol concentrations from open windrow composting facilities. Overall this has made a significant contribution to knowledge, as progress with confidently estimating bioaerosol concentrations using dispersion models has considerably improved, as highlighted in Figure 10-2.

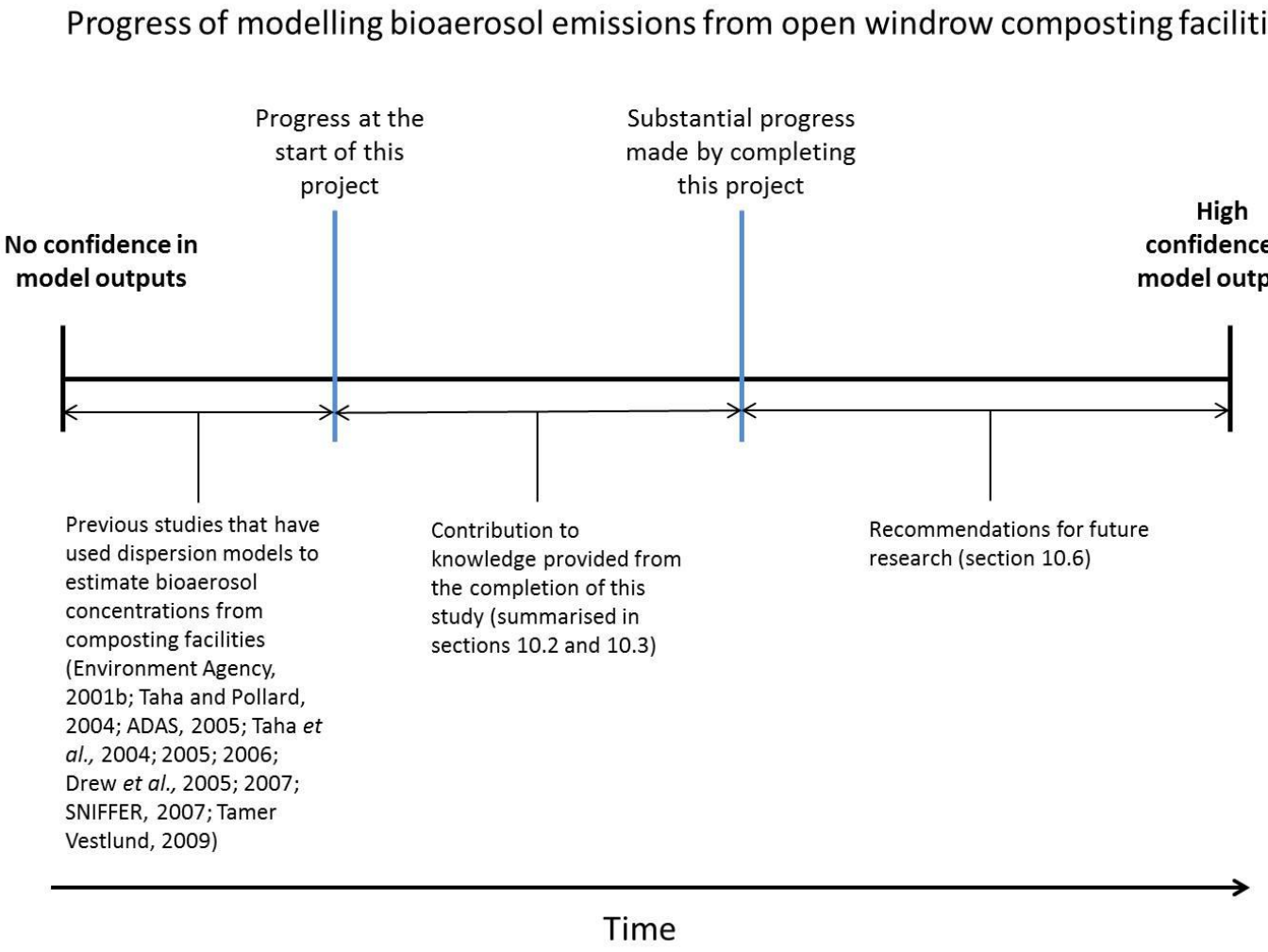

Figure 10-2 Conceptualisation of the progress made by completing this project, highlighting the contribution to knowledge made, when using dispersion models to estimate bioaerosol concentrations from open windrow composting facilities

As the completion of this project has allowed the dispersion model to be used to simulate this specific scenario more confidently, the model can now be used, albeit conservatively, to predict bioaerosol concentrations over longer timescales and wider spatial areas. This has the potential to provide a more continual indication of emissions spatially and temporally. Therefore the aim of this project, “To improve the confidence in model outputs when using dispersion models to estimate bioaerosol concentrations downwind of emissions from open windrow composting facilities” has been achieved. This has important

implications, particularly in the permitting process, as discussed further in section 10.4.

10.4 Wider implications of findings

As the model can be used with more confidence to predict bioaerosol emissions over longer time periods and larger spatial scales, it has the potential to be used to estimate bioaerosol exposure levels to nearby sensitive receptors. One gap in knowledge, briefly highlighted in Chapter 1, is associated with the level of exposure required to generate the onset of a bioaerosols-related illness. At present the 'acceptable levels' of particular bioaerosol components, proposed by the Environment Agency (Environment Agency, 2010), are precautionary levels, based on results presented in a technical report (Environment Agency, 2001a). There is no evidence to suggest that exceeding these 'acceptable levels' will result in the onset of negative health symptoms. Therefore, at present there is no solid evidence to suggest what dosage of bioaerosols emitted from open windrow composting facilities is required to generate the onset of a bioaerosols-related health problem. Using the dispersion model to estimate bioaerosol concentrations over different timescales can provide some insight into the levels of exposure experienced at the sensitive receptors. This information can be used by epidemiological experts to assess 'how much is too much'. Once these levels are established, then guidelines regarding 'acceptable' bioaerosol concentration levels at the nearest sensitive receptors can be reassessed.

Modelled concentration outputs also have the potential to be used to aid and revise the permitting process. At present certain sites are required to produce a Site Specific Bioaerosol Risk Assessment [SSBRA] (Drew *et al.,* 2009; Environment Agency, 2010) to support their permit application. This is required to show that bioaerosols will be maintained to the 'acceptable levels' at the sensitive receptors. As the dispersion model can now be used with more confidence, it has the potential to be used to assess whether bioaerosol emissions are to the stated 'acceptable levels' 250 metres from the site boundary or at the nearest sensitive receptor, in various operational and

environmental conditions. Therefore, potentially models can be used by site operators to support their permit applications. Conversely, models can also be used by the Environment Agency, the body responsible for controlling the permitting process, to prove or disprove the SSBRAs provided by the site operators, and thus accept or reject permit applications.

10.5 Limitations

Primarily, it should be recognised that dispersion modelling is a representation of reality, and will never provide exact pollutant concentrations. This should be recognised by all groups who work with dispersion model outputs. As the limitations associated with each section are stated at the end of the relevant chapter, the main limitations of this research are summarised below:

1. Limitations associated with the screening SA stage (Chapter 3)

The purpose of the screening stages was to reduce the amount of data included in the main SA. This included reducing the amount of meteorological data and, to be included in the main SA. Therefore the interaction between the meteorological inputs and remaining model inputs was not fully analysed. Additionally, an OAT method was used to reduce the parameter ranges of selected model inputs. As OAT methods do not analyse potential parameter input interactions, it is possible that sensitive ranges, which appeared to be non-sensitive, were excluded from the main SA.

2. Lack of knowledge and data surrounding input values when using the dispersion model in the open windrow composting context.

After completing an extensive literature review, it was apparent that the majority of parameter values inputted into the dispersion model in previous studies were not measured or justified, and hence it was assumed that they were guessed without reasoning. This had implications in Chapters 3 to 7, as the SA and model calibration and validation was completed by inputting, or modifying parameter values within a range or criteria relevant to the composting scenario. Assumptions regarding these ranges and criteria were completed with little evidence, therefore it is unclear whether the ranges used in these chapters

were wholly relevant to the composting scenario, or if ranges applicable to this scenario have not been included.

3. Accuracy of the sampled data

The model calibration and validation was completed using measured data collected using SKC personal filter samplers (SKC Inc., 2012), as was the measured bioaerosol concentration data in Chapter 8. The main limitation of this culture-based method is that nonviable or viable-but-non-culturable components are not accounted for, although these elements are still associated with negative health effects (Swan *et al.,* 2003). This potentially produces a sampled dataset which underestimated actual bioaerosol concentrations. Therefore, potentially, the model tests, sampled data and emission rate calculations presented in this thesis are underestimations of reality. This may have serious implications when using the model to estimate bioaerosol exposure levels as discussed in section 10.4. Additionally SKC samplers have a high LLOD, often resulting in more apparent 'zero' concentration values. However, the sampled dataset used to complete the model calibration and validation is the most extensive and detailed dataset available. This sampling method was also the most appropriate for the purpose of this study, at the time of measurement. Additionally, it is only possible to use this sampling method in dry weather conditions. Consequently, this has affected the model recommendations, as it is only possible to provide model recommendations when simulating bioaerosol emissions in dry weather conditions.

As there is a lack of extensive sampled datasets, it was only possible to validate the model using data collected from one open windrow composting facility. Ideally, to ensure full confidence in the model set-up, the model would have been tested against several datasets, but was not possible in the timescale of this project.

During the selected model input parameter quantification improvements, the main assumption was that the visible pollutant plume contained the maximum concentrations of bioaerosols. If this assumption is not correct, the pollutant

temperature and pollutant exit velocity measurements will be erroneous. The pollutant velocity estimations were also subject to human error.

4. Order of objective completion

The structure of this thesis has been based on order in which the individual objectives were completed. Figure 10-1 illustrates how the selected input parameter quantification improvements, presented in Chapter 8, influenced decisions in Chapter 3 to 7 and vice versa. Ideally, the model calibration and validation tests would have been completed after the selected model input parameter quantification improvements. This would have allowed the model to have been calibrated and validated using more justified input values. Therefore, ideally, the work required to complete this thesis would have followed the structure illustrated in Figure 10-3.

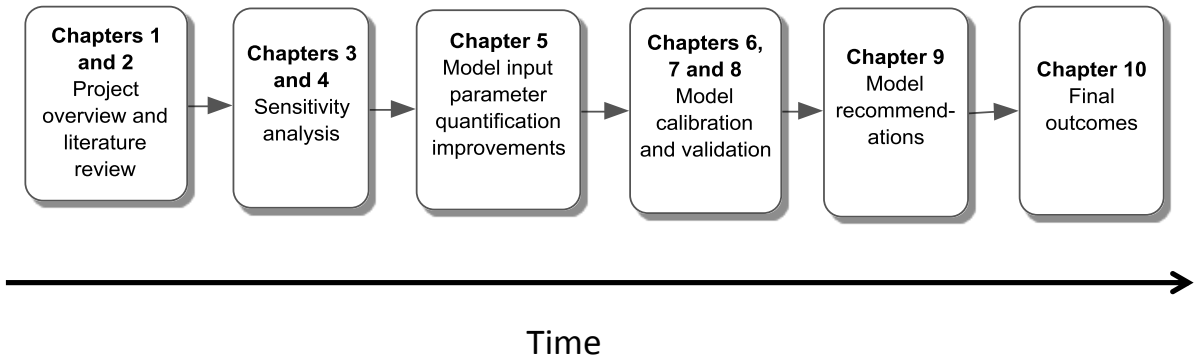

Figure 10-3 Illustration of the ideal order of the work produced for this thesis

10.6 Recommendations for future research

This project has been completed using the ADMS dispersion model. As highlighted in sections 2.4 and 3.2, there are many other different types of dispersion model that are widely used and widely available when simulating pollutant dispersal. ADMS was considered to be the most appropriate model for simulating this complex and unique scenario, at this time. However, modellers may want to consider using different dispersion models, possibly progressing to

more complex models in the future. To allow confidence in the modelled outputs when using alternative dispersion models, further tests are required. At present it is suggested in Chapter 8 that any alternative dispersion models are used alongside ADMS. It may be necessary to complete a further SA and model calibration and validation tests on the alternative model, depending on how the alternative model compares to ADMS.

The limitations highlighted in section 10.5 can be addressed be following the suggestions listed below:

- Potential improvements to the SA

The main limitation of the screening stages was the fact that any potential interactions between the meteorological input parameters and the remaining input parameters may have been overlooked. Therefore it is recommended that future SAs include altering meteorological inputs alongside the remaining parameters. This is technically difficult, depending on the number of iterations involved. This technique would be easier by entering meteorological data in the main model interface. However, a maximum of 99 different sets of meteorological data are allowed, so it may be necessary to run the SA in a series of batches. The main limitation of the SA exercise overall, was associated the lack of information and data used to justify the model inputs and input parameter ranges included within the analysis. Although the ranges were justified based on the information available at the time, it may be required to change these ranges, once further information is acquired. This would refine the SA, ensuring that the inputs included are specific to the open windrow composting context. This would also affect any additional model calibration improvements, as the input adjustments could be completed within the more refined input ranges. Additionally, a different random number generation method could be used throughout the SA, to avoid ambiguous results (Ibbotson Associates, 2005). Therefore another technique such as Latin Hypercube Sampling (McKay *et al.,* 2000; Griensven *et al.,* 2006), Fourier Amplitude Sensitivity Testing [FAST] (Helton, 1993; Xu and Gertner, 2011), or High

Dimensional Model Representation [HDMR] (Rabitz *et al.*, 1999; Li *et al.,* 2011) could be tested.

- Potential improvements to the model calibration and validation

Collecting more bioaerosol concentration data on-site would allow more extensive model calibration and validation tests to be performed in the future. Although the most extensive datasets available were used in this study, the datasets are still limited, as they were collected over a short timescales, as detailed in sections 5.2 and 6.2. There are numerous methods for monitoring bioaerosols, and many different sampling strategies could be adopted to provide an extensive dataset to validate the model. Ideally a continuous dataset whereby bioaerosols are measured at regular intervals over a long timescale would be used to validate the model, allowing the model performance to be assessed over longer time periods and differing site and meteorological conditions. Additionally, the model could be further validated using data collected at numerous sites. A recent unpublished study has been completed whereby repeated bioaerosol measurements have been taken at three different open windrow composting facilities (Defra project WR1121). The data from projects such as this could be used to further validate the model at multiple sites, to test that the current optimal model input values, are applicable when applied to other open windrow composting facilities.

As the current model recommendations are based on modelling *Aspergillus fumigatus* concentrations only, it is also recommended that the model calibration and validation tests are completed again for other bioaerosol components, such as Total Bacteria and Gram-negative Bacteria. Further work is also required to be able to use the model with confidence to predict concentrations during wet weather conditions. This was highlighted in section 9.5, as part of the model recommendations. Therefore further validation studies are required using data collected for other bioaerosol components (already available) and during wet weather conditions (not yet possible using current sampling techniques).

Although the model validation was performed using data collected from a site surrounded by buildings, further tests are recommended regarding the buildings options within the dispersion model. The use of the buildings module exacerbated the correspondence between the modelled and sampled data. However, this is thought to have been caused due to the restrictions of the dispersion model, as the buildings option cannot be used with an area source. Once the model developers have addressed this issue, it is recommended that the use of the buildings options is tested again.

- Potential improvements to the model input parameter quantification exercise

More input parameters need to be quantified to justify the inputs and input ranges used within the dispersion model. Additionally more measurements from more sites, during different weather conditions and agitation activities are required to assess the variability of the data collected. This will ensure that model input ranges specific to the open windrow composting scenario are considered and tested. When quantifying the pollutant exit velocity, the method used was subject to human error. To improve upon this method, to allow more accurate measurements of this parameter, it is recommended that alternative measurement techniques are used .For example, placing a piece of equipment that emits an object at a known exit velocity close to the pollutant plume could allow a more accurate estimation of the pollutant exit velocity, by comparing the velocity of the bioaerosol pollutant to an object of known velocity. This may be achievable using a bubble or smoke machine. Additionally, it may be more accurate to use this technique during agitation activities performed indoors, so that ambient wind speeds do not influence the results. When collecting concentration data at the source of bioaerosol emissions caused by agitation activities, it was only possible to collect data at one point per agitation activity. Additionally, certain agitation actions were not considered, such as vehicle movements. Therefore it is recommended, that more samples are collected surrounding the whole of the agitation activity. This may be possible by attaching the sampling heads to equipment that extends across the whole of the agitation activity area, or attaching the equipment to the machinery itself. This

will provide a better overview of emissions from an agitation activity, by considering the activity as a whole, instead of a singular action.

- Emission rate

Emission rate calculations were completed using measured bioaerosol concentration data, collected at the source of the emission, in Chapter 8. However these emission rates cannot yet be used in the dispersion model with confidence, as there is no data collected downwind of the composting facility to compare modelled outputs to, as discussed in section 10.2.5. Therefore more measured data is required to allow emission rates calculated using the methods detailed in section 8.7 to be tested.

Section 10.2.5 also highlighted the variability of the emission rates used throughout this study and previous studies. As the emission rate variability is so large, it is recommended that further model tests are completed in an attempt to narrow this range. For example, the range of emission rates used in previous studies range between $6.0x10^{-6}$ $g/m^2/s$ (ADAS, 2005) to $6.7x10^{10}$ particles per second (Millner *et al.,* 1980). However, the range of emission rates used and calculated throughout this study range between $1.53x10^3$ $CFU/m^2/s$ to $1.41x10^7$ CFU/s, which somewhat correspond to the emission rates back calculated by the Environment Agency (2012) which ranged between approximately$1x10^4$ and $1x10^9$ CFU/s. Therefore, this may indicate that an emission rate falling within the middle of this range is most appropriate when modelling bioaerosol emissions in the open windrow composting context. Alternatively lower and higher emission rates, representing 'best' and 'worst' case scenarios be used. One way to test this notion would be to assign a probability distribution to the emission rates used in previous modelling studies (including this study). Then random emission rate values could be generated within this probability distribution, and used in the dispersion model. The generated model outputs could then be compared and analysed to measured data to determine which emission rates resulted in the best correspondence between the measured and modelled outputs in the majority of cases.

- Wider implications

As already discussed in section 10.4, the dispersion model can be used to predict bioaerosol exposure levels at nearby sensitive receptors. Therefore it is recommended that bioaerosol concentrations at the sensitive receptors are modelled during different scenarios, meteorological conditions and timescales, to assess the levels of exposure at different receptors, and groups of people. Furthermore, additional tests are required to test the performance of the model when predicting emissions from sites wishing to expand (sections 9.5 and 9.6). This can be completed by predicting concentrations based on information collected from existing sites, and then comparing the results to actual measured data collected from the proposed site once completed and operational.

The completion of this project has substantially improved the understanding of modelling approaches when simulating the dispersion of bioaerosols emitted from open windrow composting facilities. Although the completion of this project has allowed the model to be used with more confidence, allowing more reliable bioaerosol concentration estimates over longer timescales and wider spatial areas in the open windrow composting context, there is still the potential to complete additional tests to further develop the knowledge and understanding of the emission, dispersal and the effects of bioaerosols from open windrow composting facilities on public health.

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APPENDICES

Appendix 1 – Input values used within the dispersion model during screening stages 1 and 2 (sections 3.4.1 and 3.4.2 respectively)

All input values held constant within the dispersion model during the sensitivity analysis screening stages were based on values used in previous modelling studies when simulating bioaerosol emissions from composting facilities (Millner *et al.,* 1980; Danneberg *et al.,* 1997; Dowd *et al.,* 2000; Environment Agency, 2001b; Taha and Pollard 2004; Drew *et al.,* 2005; 2007; Taha *et al.,* 2006; 2007; SNIFFER, 2007; Tamer Vestlund 2009)

Any compulsory input parameters not detailed in the table below, compulsory referring to input parameters which are required to allow the dispersion model to run, were kept at the model default parameters. Any other input parameters not detailed in the table below were not used in the model.

Model input (Units)	Value used in Screening stage 1 (Section 3.4.1)	Value used in Screening stage 2 (Section 3.4.2)
Additional input file	"CALMS" file – default values used with the exception of the 'minimum value of wind speed' which was set to 0.1m/s	Not used
Source type	Point	Point
Pollutant specific heat capacity (J/°C/kg)	1012, the model default value	800-2100 as detailed in Table 3-2. The actual values used are provided in the data disc
Pollutant molecular mass (g)	28.966, the model default value	15-45 as detailed in Table 3-2. The actual values used are provided in the data disc
Source height (m)	3	3
Source diameter (m)	3	3

Model input (Units)	Value used in Screening stage 1 (Section 3.4.1)	Value used in Screening stage 2 (Section 3.4.2)
Pollutant exit velocity (m/s)	2	0-100, as detailed in Table 3-2. The actual values used are provided in the data disc
Pollutant temperature (°C)	20	20
Pollutant emission rate (CFU/s)	$1x10^5$	$1x10^5$
Other pollutant characteristics	A new pollutant named 'bioaerosol' was defined, and all settings were kept at the model default values	A new pollutant named 'bioaerosol' was defined, and all settings were kept at the model default values
Latitude (°)	52	52
Surface Roughness (m)	0.2	0.2
Priestley-Taylor parameter	Default value - Advanced meteorological options were not used	0-3 as detailed in Table 3-2. The actual values used are provided in the data disc
Minimum Monin-Obukhov length (m)	Default value - Advanced meteorological options were not used	1-200 as detailed in Table 3-2. The actual values used are provided in the data disc
Surface Albedo	Default value - Advanced meteorological options were not used	0-1 as detailed in Table 3-2. The actual values used are provided in the data disc
Meteorological data	From a separate file as detailed in section 3.4.1 and Table 3-1 – actual values used are provided in the data disc	Based on the results from screening stage 1 (section 3.5.1) as detailed in Table 3-3
Model output options	Short term with an averaging time of 1 hour. Units for output: CFU/m^3	Short term with an averaging time of 1 hour. Units for output: CFU/m^3